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Recently, detailed benchmark specifications have been issued for the Light Water Breeder Reactor (LWBR) Seed and Blanket (SB) critical experiments. These benchmarks are of particular interest because they include critical lattices of ^{233}U and highly enriched uranium fuel pins completely immersed in water. All of these benchmarks have thermal spectra.

MCNP5 calculations have been performed for the eight benchmarks in the set, using ENDF/B-V and ENDF/B-VI nuclear data libraries. ENDF/B-V produces good agreement with the benchmark values for k_{eff}. ENDF/B-VI produces reasonable agreement with the benchmark values but not as good as ENDF/B-V. However, the ENDF/B-VI results are less sensitive to the H/U ratio than the ENDF/B-V results are.

Both ENDF/B-V and ENDF/B-VI substantially underpredict k_{eff} for the three cases that have $^{233}UO_2$-ThO_2 blankets. The thorium in the blanket rods contains a small amount of gadolinium, and the reactivity worth of the gadolinium varies from approximately -0.002 Δk to approximately -0.004 Δk for the three cases. Given the ambiguity in the gadolinium content and its reactivity impact, it is recommended that the uncertainty associated with the benchmark value of k_{eff} for these three cases be increased.

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Both ENDF/B-V and ENDF/B-VI substantially underpredict k_{eff} for the three cases that have $^{233}UO_2$-ThO_2 blankets. The thorium contains a small amount of gadolinium, and the calculated reactivity worth of that gadolinium ranges from approximately -0.002 Δk to approximately -0.004 Δk for the three cases. Given the ambiguity in the gadolinium content and its reactivity impact, it is recommended that the uncertainty in the benchmark value of k_{eff} be increased for these three cases.

KEYWORDS: ***^{233}U, HEU, Criticality, Thermal, Benchmarks, MCNP***

1. Introduction

The Light Water Breeder Reactor (LWBR) Seed and Blanket (SB) critical experiments were conducted by Bettis Atomic Power Laboratory in the 1960s [1]. Recently, detailed benchmark specifications have been issued for them [2]. These benchmarks are of particular interest because they include critical lattices of ^{233}U and highly enriched uranium (HEU) fuel pins completely immersed in water. All of the benchmarks have thermal spectra.

The configurations of the eight benchmarks are indicated in Figures 1and 2, with the seed pins shown in red. The horizontal black bars in the Figures indicate the location of a bank of four control rods, which was slightly inserted into the cores to obtain criticality. The seed fuel pins contained approximately 28 wt.% UO_2 in a ZrO_2 matrix, with the uranium enriched to either 97.29 wt.% in

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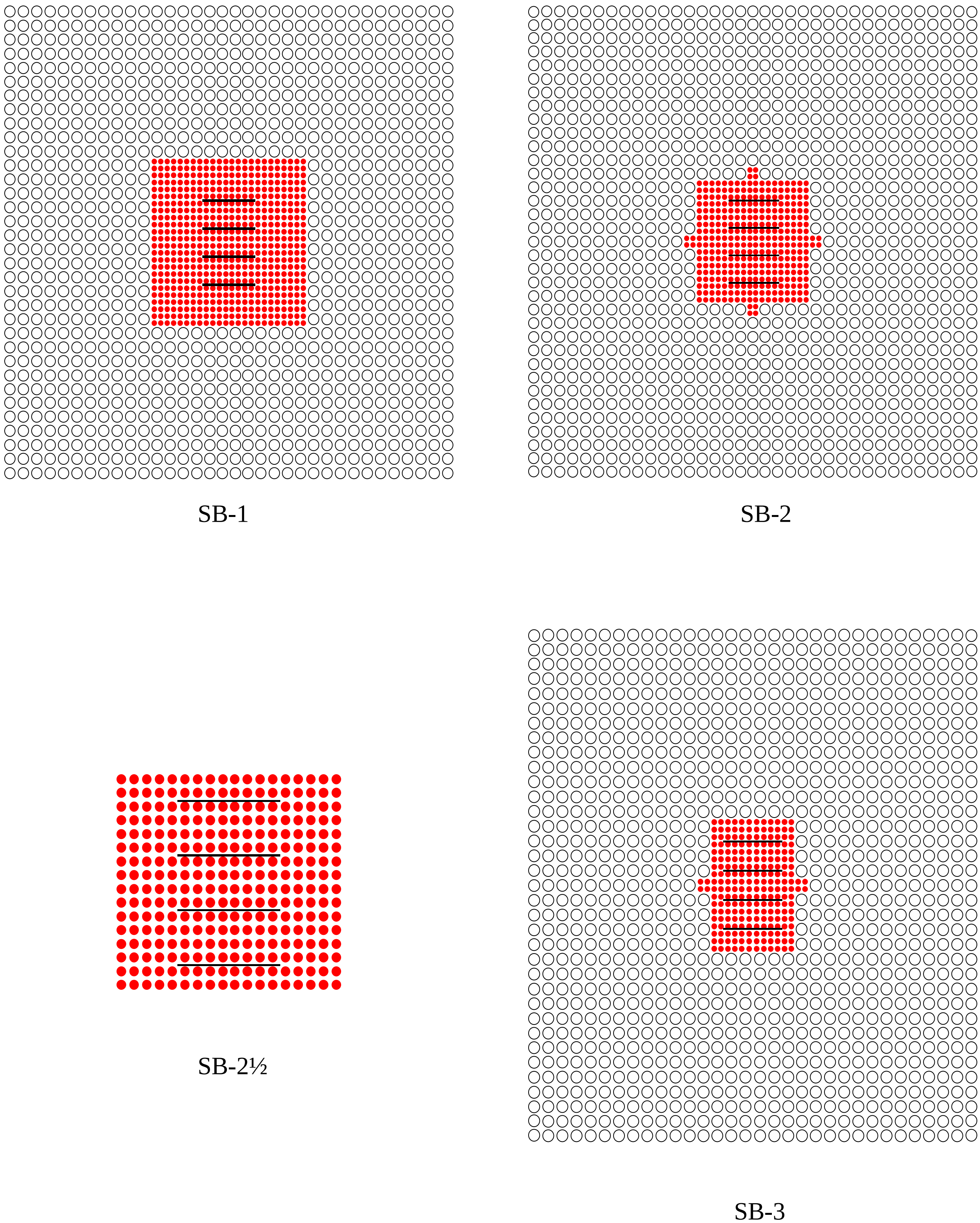

Fig. 1 Layout of Cores SB-1 through SB-3.

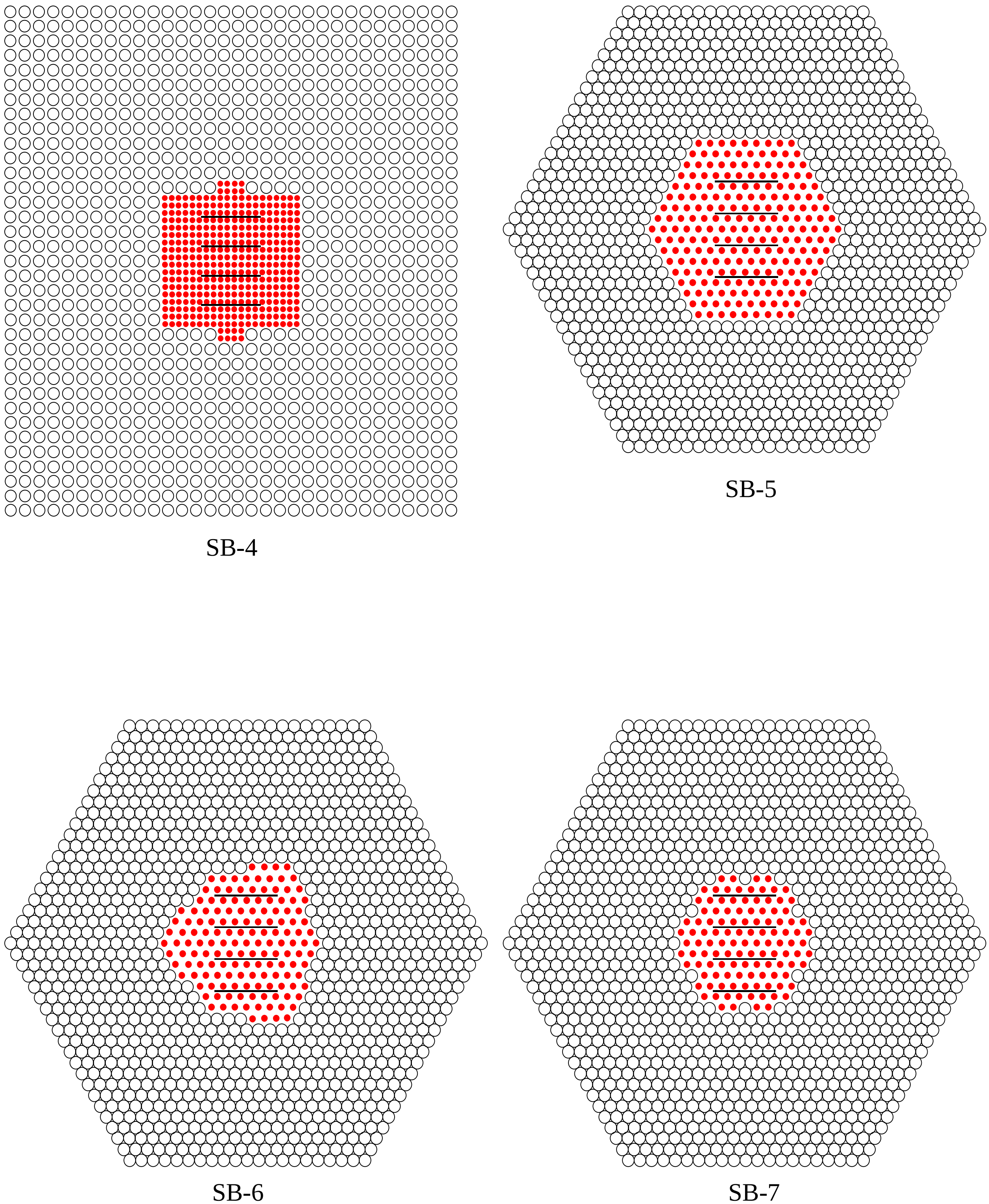

Fig. 2 Layout of Cores SB-4 through SB-7.

^{233}U or 92.73 wt.% in ^{235}U. The blanket pins contained either ThO_2 or a mixture of ThO_2 and approximately 1 wt.% UO_2, with the uranium enriched to 97.19 wt.% in ^{233}U. The seed pins had an outer fuel radius of 0.26797 cm, while the blanket pins had an outer radius of 0.62103 cm. More details about the benchmarks are provided in Table 1.

2. Calculations and Results

Calculations were performed for each benchmark with the MCNP5 Monte Carlo code [3] and nuclear data libraries derived from ENDF/B-V [4] and ENDF/B-VI [5]. The ENDF/B-VI calculations used a combination of nuclides from the ACTI [6] and ENDF66 [7] nuclear data libraries. This combination does not correspond to the final ENDF/B-VI specification for every nuclide in the calculation, but it does for hydrogen, oxygen, thorium, and all the uranium isotopes. Each calculation employed 350 generations with 10,000 neutron histories per generation, and the results from the first 50 generations were discarded. Consequently, each result is based on 3,000,000 active histories.

2.1 Results for Benchmarks

The results from these calculations are presented in Table 2, and the resulting reactivity differences are shown in Table 3. The calculated results tend to be lower than the benchmark values: six of the calculated values for k_{eff} are within one standard deviation of the corresponding benchmark value, but the other ten all are more than one standard deviation below it.

Overall, ENDF/B-V produces markedly better agreement with the benchmark values than ENDF/B-VI does. Specifically, four of the ENDF/B-V results are within one standard deviation of the benchmark value, and seven of them are within two standard deviations. Furthermore, the one case that differs by more than two standard deviations (SB-7) just barely does so. In addition, for

Table 1. Summary of LWBR SB Cores.

Case	Lattice	Rod Material		Rods		Pitch (cm)	
		Seed	Blanket	Seed	Blanket	Seed	Blanket
SB-1	Rectangular	$^{235}UO_2$-ZrO_2	ThO_2	576	1012	0.91948	1.83896
SB-2	Rectangular	$^{233}UO_2$-ZrO_2	ThO_2	340	1140	0.91948	1.83896
SB-2½	Rectangular	$^{233}UO_2$-ZrO_2	—	288	0	0.91948	—
SB-3	Rectangular	$^{233}UO_2$-ZrO_2	$^{233}UO_2$-ThO_2	224	1064	0.91948	1.83896
SB-4	Rectangular	$^{235}UO_2$-ZrO_2	$^{233}UO_2$-ThO_2	376	1026	0.91948	1.83896
SB-5	Hexagonal	$^{235}UO_2$-ZrO_2	ThO_2	217	1044	1.45034	1.45034
SB-6	Hexagonal	$^{233}UO_2$-ZrO_2	ThO_2	148	1113	1.45034	1.45034
SB-7	Hexagonal	$^{233}UO_2$-ZrO_2	$^{233}UO_2$-ThO_2	115	1146	1.45034	1.45034

Table 2 MCNP5 Results for LWBR SB Benchmarks.

Case	Benchmark k_{eff}	Calculated k_{eff}	
		ENDF/B-VI	ENDF/B-V
SB-1	1.0006 ± 0.0027	0.9963 ± 0.0005	0.9988 ± 0.0005
SB-2	1.0015 ± 0.0025	0.9993 ± 0.0006	1.0013 ± 0.0006
SB-2½	1.0000 ± 0.0024	0.9959 ± 0.0006	1.0010 ± 0.0006
SB-3	1.0007 ± 0.0025	0.9945 ± 0.0005	0.9972 ± 0.0005
SB-4	1.0015 ± 0.0026	0.9945 ± 0.0004	0.9966 ± 0.0005
SB-5	1.0015 ± 0.0028	0.9968 ± 0.0006	0.9966 ± 0.0005
SB-6	0.9995 ± 0.0027	0.9983 ± 0.0006	0.9977 ± 0.0006
SB-7	1.0004 ± 0.0028	0.9931 ± 0.0005	0.9947 ± 0.0005

Table 3 Reactivity Differences for LWBR SB Benchmarks.

Case	Benchmark k_{eff}	Δk	
		ENDF/B-VI	ENDFB-V
SB-1	1.0006 ± 0.0027	-0.0043 ± 0.0027	-0.0018 ± 0.0027
SB-2	1.0015 ± 0.0025	-0.0022 ± 0.0026	-0.0002 ± 0.0026
SB-2½	1.0000 ± 0.0024	-0.0041 ± 0.0025	0.0010 ± 0.0025
SB-3	1.0007 ± 0.0025	-0.0062 ± 0.0025	-0.0035 ± 0.0025
SB-4	1.0015 ± 0.0026	-0.0070 ± 0.0026	-0.0049 ± 0.0026
SB-5	1.0015 ± 0.0028	-0.0047 ± 0.0029	-0.0049 ± 0.0028
SB-6	0.9995 ± 0.0027	-0.0012 ± 0.0028	-0.0018 ± 0.0028
SB-7	1.0004 ± 0.0028	-0.0073 ± 0.0028	-0.0057 ± 0.0028

the six cases where one or the other of the results differs from the benchmark value by more than one standard deviation, the ENDF/B-V result is superior to the ENDF/B-VI result in five of the cases, and they are statistically indistinguishable in the remaining case. In contrast, only two of the

ENDF/B-VI results are within one standard deviation of the corresponding benchmark value, and only five of them are within two standard deviations.

At the same time, the ENDF/B-VI results are more consistent. The ENDF/B-VI results for the hexagonal cores are very similar to those for the corresponding rectangular cores, while the ENDF/B-V results for the hexagonal cores are lower than those for the corresponding rectangular cores by approximately -0.0025 Δk to -0.0050 Δk. The H/U ratio for the seed region is approximately 2.5 times higher for the hexagonal cores than for the rectangular ones. Consequently, the results in Tables 2 and 3 indicate that the ENDF/B-VI values for k_{eff} are less sensitive to the H/U ratio than the ENDF/B-V values are.

2.2 Gadolinium Worth and Sensitivity

Both ENDF/B-V and ENDF/B-VI substantially underpredict k_{eff} for the three cases that have $^{233}UO_2$-ThO_2 blankets (SB-3, SB-4, and SB-7). The thorium in the blanket rods contains a small amount of gadolinium. Unfortunately, no definitive measurement of the gadolinium content in the blanket rods was available. The gadolinium content given in the benchmark specifications is based on information from a table in the report that describes the fabrication of the fuel rods for these experiments [8]. Specifically, the benchmark specifications contain 2.9 ± 0.5 ppm of gadolinium in the thorium of the ThO_2 rods and 5.0 ± 0.5 ppm of gadolinium in the thorium of the $^{233}UO_2$-ThO_2 rods. However, the benchmark evaluation also states that gadolinium "was present in thorium feed at 1 to 10 ppm" [9].

Preliminary sensitivity calculations indicated that the gadolinium impurity produces significant reactivity changes for those three cases. Consequently, MCNP5 calculations were performed for the seven cases with ThO_2 or $^{233}UO_2$-ThO_2 blankets. The results are presented in Table 4.

The gadolinium has no significant reactivity impact for cases with ThO_2 blankets, because those blanket rods contain no fissile material. However, the gadolinium worth is quite significant for the cases with $^{233}UO_2$-ThO_2 blankets, because a substantial fraction of the fissions occurs in the blanket rods. Approximately 50% of all fissions occur in the blanket region for SB-3, approximately 45% for SB-4, and approximately 33% for SB-7. Omission of the gadolinium markedly improves the agreement between the calculated and benchmark values for k_{eff} for each of those cases, for both ENDF/B-V and ENDF/B-VI.

Th ambiguity in the gadolinium concentration, in conjunction with its reactivity impact, suggests that the uncertainty in the benchmark value of k_{eff} for cases 3, 4, and 7 should be increased. If, for example, that uncertainty were increased to ± 5.0 ppm, the benchmark values for those three cases would change as shown in Table 5, based on the ENDF/B-VI results from Table 4.

3. Summary and Conclusions

MCNP5 calculations have been performed for eight thermal benchmarks with seed cores of HEU or ^{233}U fuel pins immersed in water. The seed core is surrounded by a blanket region containing ThO_2 or $^{233}UO_2$-ThO_2 rods in seven of those benchmarks. Nuclear data based on ENDF/B-V produce good agreement with the benchmark values for k_{eff}. Nuclear data based on ENDF/B-VI produce reasonable agreement with the benchmark values but not as good as those based on ENDF/B-V. However, ENDF/B-VI produces more consistent results between the hexagonal cores and their rectangular counterparts, indicating that the ENDF/B-VI results are less sensitive to the H/U ratio than the ENDF/B-V results are.

Table 4 Gadolinium Worth for LWBR SB Benchmarks.

Case	Blanket	Library	k_{eff}, Gd	k_{eff}, No Gd	Δk_{Gd}
SB-1	ThO_2	ENDF/B-V	0.9988 ± 0.0005	0.9992 ± 0.0005	-0.0004 ± 0.0007
		ENDF/B-VI	0.9963 ± 0.0005	0.9972 ± 0.0006	-0.0008 ± 0.0008
SB-2	ThO_2	ENDF/B-V	1.0013 ± 0.0006	1.0008 ± 0.0006	0.0005 ± 0.0009
		ENDF/B-VI	0.9993 ± 0.0006	0.9992 ± 0.0006	0.0001 ± 0.0009
SB-3	$^{233}UO_2$-ThO_2	ENDF/B-V	0.9972 ± 0.0005	1.0017 ± 0.0005	-0.0045 ± 0.0007
		ENDF/B-VI	0.9945 ± 0.0005	0.9977 ± 0.0005	-0.0032 ± 0.0007
SB-4	$^{233}UO_2$-ThO_2	ENDF/B-V	0.9966 ± 0.0005	1.0002 ± 0.0005	-0.0036 ± 0.0007
		ENDF/B-VI	0.9945 ± 0.0004	0.9980 ± 0.0005	-0.0035 ± 0.0006
SB-5	ThO_2	ENDF/B-V	0.9965 ± 0.0005	0.9967 ± 0.0005	-0.0002 ± 0.0008
		ENDF/B-VI	0.9968 ± 0.0006	0.9967 ± 0.0005	0.0001 ± 0.0008
SB-6	ThO_2	ENDF/B-V	0.9977 ± 0.0005	0.9975 ± 0.0006	0.0003 ± 0.0008
		ENDF/B-VI	0.9983 ± 0.0005	0.9988 ± 0.0006	-0.0005 ± 0.0008
SB-7	$^{233}UO_2$-ThO_2	ENDF/B-V	0.9947 ± 0.0005	0.9964 ± 0.0005	-0.0017 ± 0.0007
		ENDF/B-VI	0.9931 ± 0.0005	0.9952 ± 0.0006	-0.0021 ± 0.0008

Table 5 Impact of Uncertainty in Gd Concentration on Reactivity for LWBR SB Benchmarks.

	Benchmark k_{eff}	
Case	± 0.5 ppm Gd	± 5.0 ppm Gd
SB-3	1.0007 ± 0.0025	1.0007 ± 0.0038
SB-4	1.0015 ± 0.0026	1.0015 ± 0.0041
SB-7	1.0004 ± 0.0028	1.0004 ± 0.0034

Omitting gadolinium from the blanket pins appreciably improves the agreement with the benchmark values for cases SB-3, SB-4, and SB-7 for both ENDF/B-V and ENDF/B-VI. Given the ambiguity in the gadolinium content and its reactivity impact, it is recommended that the uncertainty associated with the benchmark value of k_{eff} be increased for these three cases.

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References

1) S. Milani and S. H. Weiss, "Small Uranium-233 Fueled Seed-and-Blanket Critical Experiments," WAPD-TM-614, Bettis Atomic Power Laboratory (November 1967).
2) Valerie L. Putman, "LWBR SB Core Experiments," U233-COMP-THERM-001, *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, NEA/NSC/DOC(95)03, OECD Nuclear Energy Agency (Rev., 2003).
3) X-5 Monte Carlo Team, "MCNP — A General Monte Carlo N-Particle Transport Code, Version 5, Volume I: Overview and Theory," LA-UR-03-1987, Los Alamos National Laboratory (April 2003).
4) R. Kinsey, Ed., "ENDF-201, ENDF/B Summary Documentation," BNL-NCS-17541, 3rd Edition, Brookhaven National Laboratory (1979).
5) P. F. Rose, Ed., "ENDF-201, ENDF/B-VI Summary Documentation," BNL-NCS-17541, 4th Edition, Brookhaven National Laboratory (October 1991).
6) Stephanie C. Frankle, Robert C. Reedy, and Phillip G. Young, "ACTI: An MCNP Data Library for Prompt Gamma-Ray Spectroscopy," Proc. 12th Biennial Topl. Mtg. Radiation Protection and Shielding Div., Santa Fe, New Mexico, April 14-18, 2002 (2002).
7) Joann M. Campbell, Stephanie C. Frankle, and Robert C. Little, "ENDF66: A Continuous-Energy Neutron Data Library for MCNP4C," Proc. 12th Biennial Topl. Mtg. Radiation Protection and Shielding Div., Santa Fe, New Mexico, April 14-18, 2002 (2002).
8) W. L. Frankhouser, H. H. Crain, R. L. Fischer, J. H. Suldan, J. H. Eyler, and E. L. Speer, "Fabrication of Fuel Rods Containing U-233 Pelletized Oxide Fuels," WAPD-TM-588, Bettis Atomic Power Laboratory (February 1967). See Table 4.
9) Valerie L. Putman, *op. cit*. See Section 1.3.