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ENDF/B-VII.0, ENDF/B-VI, JEFF-3.1, AND JENDL-3.3 RESULTS FOR UNREFLECTED PLUTONIUM SOLUTIONS AND MOX LATTICES (u)

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ABSTRACT

Previous studies have indicated that ENDF/B-VII preliminary releases β-2 and β-3, predecessors to the recent initial release of ENDF/B-VII.0, produce significantly better overall agreement with criticality benchmarks than does ENDF/B-VI. However, one of those studies also suggestes that improvements still may be needed for thermal plutonium cross sections. The current study substantiates that concern by examining criticality benchmarks for unreflected spheres of plutonium-nitrate solutions and for slightly and heavily borated mixed-oxide (MOX) lattices. Results are presented for the JEFF-3.1 and JENDL-3.3 nuclear data libraries as well as ENDF/B-VII.0 and ENDF/B-VI. It is shown that ENDF/B-VII.0 tends to overpredict reactivity for thermal plutonium benchmarks over at least a portion of the thermal range. In addition, it is found that additional benchmark data are needed for the deep thermal range

Key Words: ENDF/B-VII.0, ENDF/B-VI, JEFF-3.1, JENDL-3.3, Benchmarks, Plutonium Solutions, MOX

1. INTRODUCTION

Previous studies have indicated that ENDF/B-VII preliminary releases β-2 and β-3 produce significantly better agreement with criticality benchmarks than does ENDF/B-VI. At the same time, one recent study [1] also suggests that improvements still may be needed for thermal plutonium cross sections. That suggestion, however, is based on results from just three benchmarks. This study extends that set of results to seven unreflected spheres of plutonium-nitrate solutions and to six mixed-oxide (MOX) lattices. Those 13 cases include the three from the previous study. In addition, the scope of the study has been extended to include the JEFF-3.1 and JENDL-3.3 nuclear data libraries as well as ENDF/B-VII.0 and ENDF/B-VI.

All of the experiments upon which the benchmarks are based were performed at the Critical Mass Laboratory of Pacific Northwest Laboratories (PNL). Specifications for all of the benchmarks are taken from the *International Handbook of Evaluated Criticality Benchmark Experiment* [2]. All but one of them also are designated as benchmarks by the Cross Section Evaluation Working Group (CSWEG) [3]. The CSEWG identifiers have been retained herein, principally because they are more compact than the full *Handbook* identifiers. Table I provides a succinct description of the 13 benchmarks.

Table I. Succinct Description of Benchmarks

Name	*Handbook* ID	Description
PNL-1	PU-SOL-THERM-021, case 7	unreflected 14-inch sphere of plutonium nitrate
PNL-3	PU-SOL-THERM-011, case 18-1	unreflected 18-inch sphere of plutonium nitrate
PNL-4	PU-SOL-THERM-011, case 18-6	unreflected 18-inch sphere of plutonium nitrate
PNL-5	PU-SOL-THERM-011, case 16-5	unreflected 16-inch sphere of plutonium nitrate
PNL-6	PU-SOL-THERM-021, case 3	unreflected 15.2-inch sphere of plutonium nitrate
PNL-8	PU-SOL-THERM-021, case 2	unreflected 15.2-inch sphere of plutonium nitrate
PST-9	PU-SOL-THERM-009, case 3a	unreflected 48-inch sphere of plutonium nitrate
PNL-30	MIX-COMP-THERM-002, case 30	lattice of 469 MOX pins, pitch=1.77800 cm
PNL-31	MIX-COMP-THERM-002, case 31	lattice of 761 MOX pins, pitch=1.77800 cm
PNL-32	MIX-COMP-THERM-002, case 32	lattice of 195 MOX pins, pitch=2.20914 cm
PNL-33	MIX-COMP-THERM-002, case 33	lattice of 761 MOX pins, pitch=2.20914 cm
PNL-34	MIX-COMP-THERM-002, case 34	lattice of 161 MOX pins, pitch=2.51447 cm
PNL-35	MIX-COMP-THERM-002, case 35	lattice of 689 MOX pins, pitch=2.51447 cm

2. CALCULATIONS

Four sets of calculations were performed for these benchmarks using the MCNP5 Monte Carlo code [4]. The first set employed nuclear data based on ENDF/B-VII.0, which was released in December 2006. The second set used data based on the final release for ENDF/B-VI, the third set used data derived from JEFF-3.1 [5], and the fourth set used data derived from JENDL-3.3 [6]. However, the JENDL-3.3 calculations employed a thermal scattering law, $S(\alpha,\beta)$, for hydrogen in water based on ENDF/B-VI [6] because the JENDL-3.3 library distributed for MCNP does not include one.

All of the MCNP5 calculations were run with 5,000,000 active neutron histories. That number of histories is sufficient to render the statistical uncertainty from the calculations essentially negligible relative to the benchmark uncertainties.

3. UNREFLECTED SOLUTIONS OF PLUTONIUM NITRATE

Six of the unreflected spheres of plutonium-nitrate solutions are identified as PNL-1 through PNL-8, with two omissions (PNL-2 and PNL-7 are omitted, because PNL-2 is a idealization of PNL-6 and PNL-7 is reflected by water). These six cases appear in both the CSEWG benchmark book and the ICSBEP *Handbook*. The seventh case, PST-9, has a much larger radius than the other solution benchmarks and is taken from the *Handbook*. Its radius is approximately 61 cm, while the radii of the other solutions range approximately from 17 to 23 cm. Consequently, it has much lower leakage than the other solution benchmarks. All of these benchmarks involve a homogeneous sphere of plutonium-nitrate solution. For PNL-1, the sphere is bare. For all of the others, the sphere is encased in a spherical shell of aluminum or steel. For PNL-4 and PNL-5, there is a thin layer of cadmium on the outer surface of the shell. More specific details about the seven cases are given in Table II.

Table II. Characteristics of PNL $PuNO_3$ Solutions

Case	Benchmark k_{eff}	N_H/N_{Pu-239}	ENDF/B-VII.0 Leakage Fraction (%)	ENDF/B-VII.0 Fission Fraction (%)		
				Fast	Intermediate	Thermal
PNL-1	1.0000 ± 0.0032	701.70	37.4	0.4	3.4	96.2
PNL-3	1.0000 ± 0.0052	1207.8	27.8	0.3	2.2	97.5
PNL-4	1.0000 ± 0.0052	907.13	29.3	0.3	2.8	96.9
PNL-5	1.0000 ± 0.0052	574.52	37.1	0.5	4.1	95.4
PNL-6	1.0000 ± 0.0065	131.83	39.1	2.1	14.1	83.8
PNL-8	1.0000 ± 0.0032	797.62	35.0	0.4	3.1	96.5
PST-9	1.0003 ± 0.0033	2806.8	7.1	0.1	1.2	98.7

The calculated values of k_{eff} for the PNL plutonium-nitrate solutions are given in Table III, and the differences between the calculated and benchmark values are plotted in Fig. 1. The curves for the four libraries have nearly identical shapes, with the JENDL-3.3 curve displaced slightly upward from the other three. In fact, there is very little difference in the values of k_{eff} from the other three nuclear data libraries.

The shape of the curve for N_H/N_{Pu-239} atom ratios below 1200 suggests that some further refinement may be needed in thermal plutonium cross sections, especially since at least four of the seven results from each of the libraries differ from the corresponding benchmark value by more than one standard deviation. For all of those cases, the calculated value is higher than the benchmark value. Furthermore, all four libraries overestimate k_{eff} by more than one standard deviation for all three cases with ratio values between 500 and 800.

The calculated values of k_{eff} for PST-9, with an atom ratio of approximately 2800, all differ from the corresponding benchmark ratio by more than five standard deviations (the benchmark uncertainty is 0.0033 Δk). Clearly, additional benchmarks with atom ratios between 1500 and 3000 are needed to determine whether PST-9 is a valid data point or simply an outlier. Unfortunately, no such benchmarks have been identified as of yet.

4. MOX LATTICES

The MOX lattices also are denoted by their CSEWG identifiers, PNL-30 through PNL-35. The MOX pins all contain 2.0 wt.% PuO_2 with 8.0 at.% ^{240}Pu in the plutonium. They are arranged on a square lattice and are fully immersed in water. The outer diameter of each pin is 0.505 inch, and they are 36 inches long, including the bottom 0.5 cm which contains natural UO_2 rather than

Table III. MCNP5 Results for PNL $PuNO_3$ Solutions

Case	Calculated k_{eff}			
	ENDF/B-VII.0	ENDF/B-VI	JEFF-3.1	JENDL-3.3
PNL-1	**1.0066 ± 0.0004**	*1.0063 ± 0.0004*	**1.0069 ± 0.0004**	**1.0101 ± 0.0004**
PNL-3	0.9950 ± 0.0004	0.9954 ± 0.0004	0.9958 ± 0.0004	0.9985 ± 0.0004
PNL-4	1.0002 ± 0.0004	1.0012 ± 0.0004	1.0013 ± 0.0004	1.0043 ± 0.0004
PNL-5	*1.0066 ± 0.0004*	*1.0058 ± 0.0004*	*1.0067 ± 0.0004*	*1.0098 ± 0.0004*
PNL-6	1.0040 ± 0.0005	1.0029 ± 0.0005	1.0045 ± 0.0005	*1.0070 ± 0.0004*
PNL-8	*1.0052 ± 0.0004*	*1.0060 ± 0.0004*	*1.0057 ± 0.0004*	**1.0101 ± 0.0004**
PST-9	**1.0189 ± 0.0002**	**1.0190 ± 0.0002**	**1.0186 ± 0.0002**	**1.0226 ± 0.0002**

$\sigma < |\Delta k| \le 2\sigma$ **$|\Delta k| > 2\sigma$**

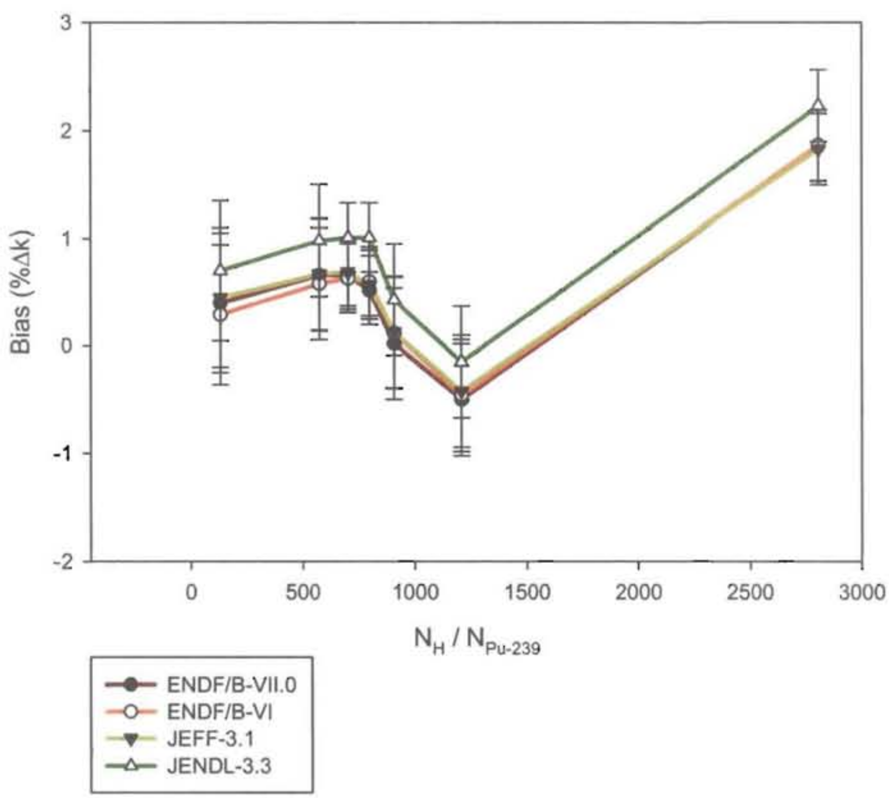

Figure 1. Results for Unreflected Plutonium-Nitrate Solutions.

MOX. The pins are clad in Zircaloy2, and the MOX density is 9.54 g/cm^3. There are two benchmarks for each of three lattice pitches (1.77800, 2.20914, and 2.51447 cm). The water for the even-numbered cases is only slightly borated, while that for the odd-numbered cases is much more heavily borated. Consequently, the even-numbered cases contain substantially fewer fuel pins than their odd-numbered counterparts. More specific details about the six cases are given in Table III.

Table III. Characteristics of PNL MOX Lattices

Case	Benchmark k_{eff}	Fuel Rods	Soluble Boron (PPM)	ENDF/B-VII.0 Leakage Fraction (%)	ENDF/B-VII.0 Fission Fraction (%)		
					Fast	Inter	Thermal
PNL-30	1.0000 ± 0.0032	469	1.7	0.77	8.6	10.3	81.1
PNL-31	1.0000 ± 0.0065	761	687.9	0.36	9.3	11.8	78.9
PNL-32	1.0000 ± 0.0052	195	0.9	1.27	5.3	5.6	89.1
PNL-33	1.0000 ± 0.0052	761	1090.4	0.23	6.3	7.2	86.5
PNL-34	1.0000 ± 0.0052	161	1.6	1.63	4.4	4.2	91.4
PNL-35	1.0000 ± 0.0025	689	767.2	0.26	5.1	5.4	89.5

The calculated values for k_{eff} for the MOX lattices are presented in Table IV, and the differences between the calculated and benchmark values are plotted in Fig. 2 and Fig. 3. Once again, the curves for the four libraries have very similar shapes, although those shapes are different for the slightly borated cases and the heavily borated cases. The corresponding values for k_{eff} obtained from ENDF/B-VII.0, JEFF-3.1, and JENDL-3.3 are in very good agreement with each other, but the results from ENDF/B-VI are noticeably lower for all six cases.

All four libraries produce a nearly straight-line bias for the slightly borated cases. In fact, a constant bias could be chosen for ENDF/B-VII.0, JEFF-3.1, or JENDL-3.3 that would still fall within a single standard deviation of the calculated results. In contrast, the biases from those three libraries for the highly borated cases exceed the corresponding benchmark value by more than a standard deviation for the middle pitch and by more than two standard deviations for the largest pitch. Furthermore, the bias is high for all six of those results.

5. SUMMARY AND CONCLUSIONS

Overall, the results for these benchmarks suggest that further refinements may be needed for thermal plutonium cross sections in future releases of ENDF/B-VII, JEFF, or JENDL.. The preponderance of cases where the calculated value for k_{eff} is higher than the corresponding

Table IV. MCNP5 Results for PNL MOX Lattices

Case	Calculated k_{eff}			
	ENDF/B-VII.0	ENDF/B-VI	JEFF-3.1	JENDL-3.3
PNL-30	1.0019 ± 0.0003	*0.9933 ± 0.0003*	1.0000 ± 0.0003	0.9987 ± 0.0003
PNL-31	1.0028 ± 0.0003	*0.9960 ± 0.0004*	1.0018 ± 0.0003	1.0008 ± 0.0004
PNL-32	1.0035 ± 0.0003	**0.9965 ± 0.0004**	1.0022 ± 0.0003	1.0018 ± 0.0004
PNL-33	**1.0072 ± 0.0003**	1.0029 ± 0.0003	**1.0072 ± 0.0003**	**1.0069 ± 0.0003**
PNL-34	1.0041 ± 0.0003	**0.9989 ± 0.0003**	1.0032 ± 0.0003	1.0033 ± 0.0003
PNL-35	*1.0069 ± 0.0003*	1.0031 ± 0.0003	*1.0057 ± 0.0003*	*1.0062 ± 0.0004*

$\sigma < |\Delta k| \leq 2\sigma$ **$|\Delta k| > 2\sigma$**

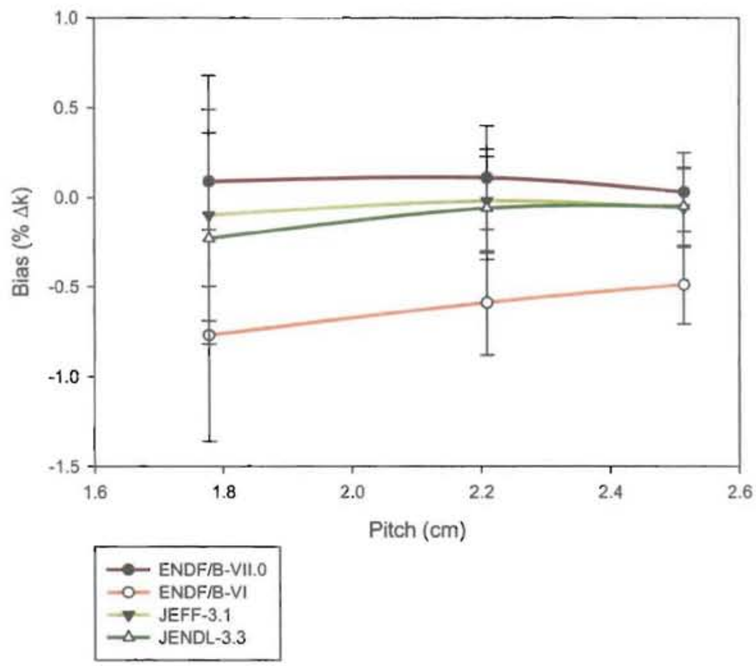

Figure 2. Reactivity Bias for Slightly Borated PNL MOX Lattices.

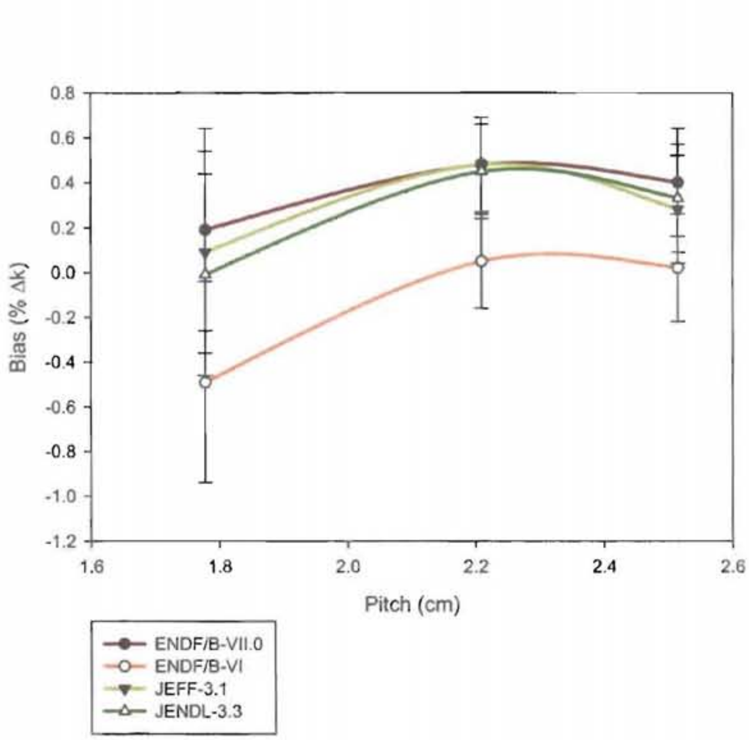

Figure 3. Reactivity Bias for Heavily Borated PNL MOX Lattices.

benchmark value by more than one standard deviation (six of the 13 cases for ENDF/B-VII.0 and JEFF-3.1, seven of the cases for JENDL-3.3) suggests that the current cross sections produce excessive reactivity over at least a portion of the thermal energy range. In addition, the very large difference between the calculated and benchmark values for k_{eff} for PST-9 clearly indicates that additional benchmark data are needed for the deep thermal range.

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