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ENDF/B-VII.0, ENDF/B-VI, JEFF-3.1, AND JENDL-3.3 RESULTS FOR THE MCNP CRITICALITY VALIDATION SUITE AND OTHER CRITICALITY BENCHMARKS

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Extended Summary

1. Nuclear Data Libraries

ENDF/B-VII.0, the initial release of the ENDF/B-VII nuclear data library (Chadwick *et al.*, 2006), was formally released in December 2006. A few months before that, a nuclear data library for the MCNP Monte Carlo code (X-5 Monte Carlo Team, 2003) derived from the JEFF-3.1 nuclear data library (Cabellos, 2006) became available, joining those previously available based on JENDL-3.3 (Kosako *et al.*, 2003) and ENDF/B-VI (X-5 Monte Carlo Team, 2003).

The study discussed herein compares results obtained for the MCNP Criticality Validation Suite and other selected criticality benchmarks using MCNP5 and those four libraries. A previously published comparison for the MCNP Criticality Validation Suite (Mosteller and MacFarlane, 2006) employed a pre-release version of ENDF/B-VII and did not include JEFF-3.1.

The MCNP5 calculations discussed herein were run with 5,000,000 active neutron histories for all but two cases. This number of histories is sufficient to render the computational uncertainty from the MCNP5 calculations essentially negligible relative to the benchmark uncertainty for most of the cases. Fewer active histories were run for those two cases because they require substantially more computer time per history than the others. Nonetheless, the computational uncertainties for k_{eff} from those two cases is comparable to those for other cases.

The JENDL-3.3 calculations for thermal cases employed thermal scattering laws based on ENDF/B-VI (Little and MacFarlane, 2003), because the distributed JENDL-3.3 library did not include them.

2. Results for the MCNP Validation Suite

The MCNP criticality validation suite is a collection of 31 benchmarks taken from the *International Handbook of Evaluated Criticality Benchmark Experiments* (International Handbook of Evaluated Criticality Benchmark Experiments, 2006). It contains cases for a variety of fuels, including ^{233}U, highly enriched uranium (HEU), intermediate-enriched uranium (IEU), low-enriched uranium (LEU), and plutonium. For each fuel type, there are cases with a variety of moderators, reflectors, spectra, and geometries. The cases in the suite are summarized in Table I.

Table I. MCNP Criticality Validation Suite.

Spectrum	Fast			Intermediate	Thermal	
Geometry	Bare	Heavy Reflector	Light Reflector	Any	Lattice of Fuel Pins in Water	Solution
^{233}U	Jezebel-233	Flattop-23	U233-MF-05 (2)*	Falstaff (1)†	SB-2½	ORNL-11
HEU	Godiva Tinkertoy-2 (c-11)	Flattop-25	Godiver	UH_3 (6) Zeus (2)	SB-5	ORNL-10
IEU	IEU-MF-03	BIG TEN	IEU-MF-04	Zebra-8H‡	IEU-CT-02 (3)	STACY-36
LEU					BaW XI (2)	LEU-ST-02 (2)
Pu	Jezebel Jezebel-240 Pu Buttons (3)	Flattop-Pu THOR	Pu-MF-11	HISS/HPG‡	PNL-33	PNL-2

* Numbers in parentheses identify a specific case within a sequence of benchmarks
† Extrapolated to critical
‡ k_{∞} measurement

The results from the calculations are presented in Table II. Overall, ENDF/B-VII.0 clearly produces the best results, which is not surprising since the other three libraries are significantly older than it is. Nineteen of the 31 ENDF/B-VII.0 results are within a single standard deviation of the corresponding benchmark value for k_{eff}, and only six of them differ by more than two standard deviations. In contrast, nine of the ENDF/B-VI and JENDL-3.3 results and twelve of the JEFF-3.1 results differ from the corresponding benchmark value by more than two standard deviations.

ENDF/B-VII.0 shows particular improvement for the ^{233}U, HEU, and plutonium cases with fast spectra relative to the three other libraries. Furthermore, there is much greater consistency between the results for the bare spheres and the corresponding Flattop cases, which surround the sphere of fissile material with normal uranium. It also produces dramatically better results for BIG TEN, a cylinder of 10 wt.% enriched uranium surrounded by normal uranium. In addition, it produces better results for the water-reflected spheres of HEU and plutonium.

Relative to ENDF/B-VI, ENDF/B-VII.0 also produces significant improvements for several cases with significant amounts of hydrogen, such ORNL-11, UH_3 (6), and BaW XI (2). This improvement is due primarily to changes in the intermediate and thermal nuclear data for ^{233}U, ^{235}U, and/or ^{238}U rather than changes to the hydrogen cross sections themselves.

Table II MCNP5 Results for Criticality Safety Validation Set.

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VII.0	ENDF/B-VI	JEFF-3.1	JENDL-3.3
Jezebel-233	1.0000 ± 0.0010	0.9996 ± 0.0003	**0.9926 ± 0.0003**	**1.0038 ± 0.0003**	**1.0041 ± 0.0003**
Flattop-23	1.0000 ± 0.0014	0.9996 ± 0.0003	1.0003 ± 0.0003	**1.0062 ± 0.0003**	0.9985 ± 0.0003
U233-MF-05 (2)	1.0000 ± 0.0030	**0.9926 ± 0.0003**	0.9972 ± 0.0003	**1.0004 ± 0.0003**	1.0019 ± 0.0003
Falstaff (1)	1.0000 ± 0.0083	*0.9845 ± 0.0005*	*0.9895 ± 0.0005*	*0.9841 ± 0.00050*	*0.9879 ± 0.0005*
SB-2½	1.0000 ± 0.0024	*1.0038 ± 0.0004*	*0.9964 ± 0.0004*	*0.9971 ± 0.0004*	0.9979 ± 0.0005
ORNL-11	1.0006 ± 0.0029	1.0015 ± 0.0002	*0.9974 ± 0.0002*	*0.9975 ± 0.0002*	0.9989 ± 0.0002
Godiva	1.0000 ± 0.0010	1.0000 ± 0.0003	**0.9963 ± 0.0003**	**0.9965 ± 0.0003**	**1.0033 ± 0.0003**
Tinkertoy-2 (c-11)	1.0000 ± 0.0038	1.0007 ± 0.0003	0.9973 ± 0.0004	0.9977 ± 0.0003	*1.0042 ± 0.0003*
Flattop-25	1.0000 ± 0.0030	1.0028 ± 0.0003	1.0021 ± 0.0003	1.0020 ± 0.0003	0.9974 ± 0.0003
Godiver	0.9985 ± 0.0011	*1.0005 ± 0.0003*	**0.9948 ± 0.0003**	**0.9946 ± 0.0003**	**1.0019 ± 0.0004**
UH_3 (6)	1.0000 ± 0.0047	0.9953 ± 0.0004	*0.9914 ± 0.0003*	*0.9942 ± 0.0004*	0.9967 ± 0.0004
Zeus (2)	0.9997 ± 0.0008	**0.9967 ± 0.0003**	**0.9942 ± 0.0003**	**0.9950 ± 0.0003**	**0.9956 ± 0.0003**
SB-5	1.0015 ± 0.0028	0.9996 ± 0.0005	0.9989 ± 0.0005	*0.9968 ± 0.0005*	1.0019 ± 0.0005
ORNL-10	1.0015 ± 0.0026	0.9993 ± 0.0002	0.9992 ± 0.0002	0.9988 ± 0.0002	0.9999 ± 0.0002
IEU-MF-03	1.0000 ± 0.0017	*1.0025 ± 0.0003*	0.9987 ± 0.0003	0.9985 ± 0.0003	*0.9969 ± 0.0002*
BIG TEN	0.9948 ± 0.0013	0.9946 ± 0.0002	**1.0071 ± 0.0003**	**0.9876 ± 0.0002**	**0.9851 ± 0.0002**
IEU-MF-04	1.0000 ± 0.0030	**1.0073 ± 0.0003**	*1.0036 ± 0.0003*	*1.0037 ± 0.0003*	1.0024 ± 0.0003
Zebra-8H	1.0300 ± 0.0025	**1.0189 ± 0.0002**	**1.0406 ± 0.0002**	**1.0156 ± 0.0002**	**1.0152 ± 0.0002**
IEU-CT-02 (3)	1.0017 ± 0.0044	1.0037 ± 0.0003	1.0004 ± 0.0003	1.0001 ± 0.0003	1.0014 ± 0.0003
STACY-36	0.9988 ± 0.0013	0.9989 ± 0.0003	0.9986 ± 0.0003	0.9991 ± 0.0003	0.9999 ± 0.0003
BaW XI (2)	1.0007 ± 0.0012	1.0012 ± 0.0003	**0.9968 ± 0.0003**	1.0004 ± 0.0003	*0.9991 ± 0.0003*
LEU-ST-02 (2)	1.0024 ± 0.0037	*0.9955 ± 0.0003*	*0.9953 ± 0.0003*	*0.9963 ± 0.0003*	*0.9963 ± 0.0003*
Jezebel	1.0000 ± 0.0020	1.0000 ± 0.0003	*0.9971 ± 0.0003*	1.0000 ± 0.0003	*0.9966 ± 0.0003*
Jezebel-240	1.0000 ± 0.0020	1.0003 ± 0.0003	0.9980 ± 0.0003	**1.0043 ± 0.0003**	1.0009 ± 0.0003
Pu Buttons (3)	1.0000 ± 0.0030	0.9989 ± 0.0003	*0.9962 ± 0.0003*	0.9996 ± 0.0003	*0.9958 ± 0.0003*
Flattop-Pu	1.0000 ± 0.0030	0.9999 ± 0.0003	1.0016 ± 0.0003	1.0019 ± 0.0003	**0.9904 ± 0.0003**
THOR	1.0000 ± 0.0006	**0.9978 ± 0.0003**	**1.0057 ± 0.0003**	**1.0020 ± 0.0003**	**1.0066 ± 0.0003**
Pu-MF-11	1.0000 ± 0.0010	1.0002 ± 0.0004	**0.9966 ± 0.0004**	**0.9970 ± 0.0003**	*0.9982 ± 0.0003*
HISS/HPG	1.0000 ± 0.0110	*1.0118 ± 0.0003*	1.0106 ± 0.0003	1.0073 ± 0.0002	*1.0134 ± 0.0003*
PNL-33	1.0024 ± 0.0021	**1.0072 ± 0.0003**	1.0029 ± 0.0003	**1.0072 ± 0.0003**	**1.0069 ± 0.0003**
PNL-2	1.0000 ± 0.0065	1.0046 ± 0.0005	1.0031 ± 0.0005	1.0045 ± 0.0004	1.0062 ± 0.0005

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

3. Other Selected Criticality Benchmarks

There are still a number of areas where results using the ENDF/B-VII.0 nuclear data library could be improved. For example, ENDF/B-VII.0 pre-release versions β-1 and β-2 produce values for THOR and

U233-MF-05 (2) that are within a single standard deviation of the corresponding benchmark value, but the final changes to the cross sections for thorium and beryllium substantially reduced the value of k_{eff} for those two cases.

Further analyses have identified a number of specific areas where improvement still is needed in the ENDF/B-VII.0 nuclear data. These areas include the unresolved resonance region for ^{235}U, fast cross sections for neptunium and copper, thermal cross sections for plutonium and cadmium, and possibly the angular scattering distribution for deuterium. Results from specific cases that highlight these deficiencies will be presented in the full paper.

4. Conclusions

ENDF/B-VII.0 produces significantly better overall results for the cases in the MCNP Criticality Validation Suite than do ENDF/B-VI, JENDL-3.3, or JEFF-3.1. However, further improvements still are needed in some areas. In particular, it is suggested that the fast cross sections for beryllium and thorium be reviewed again before the next interim version of ENDF/B-VII is issued. In additions, improvements are needed for ^{235}U in the unresolved resonance region for ^{235}U, for copper and neptunium in the fast range, for plutonium and cadmium in the thermal range, and possibly for the angular scattering distribution for deuterium.

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