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ENDF/B-VII.0, the initial release of the ENDF/B-VII nuclear data library,[1] was formally released in December 2006. A few months before that, a nuclear data library for the MCNP Monte Carlo code[2] derived from the JEFF-3.1 nuclear data library[3] became available, joining those previously available based on JENDL-3.3[4] and ENDF/B-VI.[2] The study discussed herein compares MCNP5 results obtained for the MCNP Criticality Validation Suite using those four libraries. A previously published comparison[5] employed a pre-release version of ENDF/B-VII and did not include JEFF-3.1

The MCNP criticality validation suite is a collection of 31 benchmarks taken from the *International Handbook of Evaluated Criticality Benchmark Experiments*.[6] 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.

The MCNP5 calculations were run with 5,000,000 active neutron histories for all but two cases in the suite. Only 3,000,000 active histories were used for those cases, SB-5 and Zebra-8H, because they require substantially more computer time per history than the other cases. Nonetheless, the standard deviation for k_{eff} from those cases is comparable to those for other cases in the suite. This number of histories is sufficient to render the statistical uncertainty from the MCNP5 calculations essentially negligible relative to the benchmark uncertainty for most of the cases in the suite.

The JENDL-3.3 calculations for the thermal cases employed thermal scattering laws based on ENDF/B_VI,[7] since the distributed JENDL-3.3 did not include them.

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,

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

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

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

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 other 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.

Data changes from ENDF/B-VI to ENDF/B-VII.0 produce significant reactivity changes to some cases without a meaningful improvement to the agreement with the corresponding benchmark value. Specifically, the values of k_{eff} for Zebra-8H and THOR drop so much that they go from more than two standard deviations high to more than two standard deviations low.

In some cases, pre-release versions of ENDF/B_VII produced better results than ENDF/B-VII.0 does. In particular, pre-release versions β-1 and β-2 produced values for THOR and U233-MF-05 (2) that were 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.

In conclusion, 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.

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REFERENCES

1. M. B. Chadwick, *et al.*, "ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology," *Nuclear Data Sheets*, **107**, pp. 2931-3059 (December 2006).
2. 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).
3. O. Cabellos, "Processing of the JEFF-3.1 Cross Section Library into a Continuous Energy Monte Carlo Radiation Transport and Criticality Data Library," NEA/NSC/DOC(2006)18, OECD NEA Data Bank (May 2006).
4. K. Kosako, N. Yamano, T. Fukahori, K. Shibata, and A. Hasegawa, "The Libraries FSXLIB and MATXSLIB Based on JENDL-3.3," Japan Atomic Energy Research Institute report JAERI-Data/Code 2003-011 (July 2003).
5. R. D. Mosteller and R. E. MacFarlane, "Comparison of Results for the MCNP Criticality Validation Suite Using ENDF/B-VII and Other Nuclear Data Libraries," *Proceedings of PHYSOR 2006, Advances in Nuclear Analysis and Simulation*, Vancouver, Canada (September 2006).
6. *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, OECD Nuclear Energy Agency report NEA/NSC/DOC(95)03, September 2006 Edition.
7. R. C. Little and R. E. MacFarlane, "SAB2002—An S(α,β) Library for MCNP," X-5-03-21(U), Los Alamos National Laboratory (February 3, 2003).