

LA-UR-03-0027

Approved for public release;
distribution is unlimited.

Title: Testing of the ENDF66 Nuclear Data Library with the MCNP
Criticality Validation Suite

Author(s): Russell D. Mosteller

Submitted to: 2003 Annual Meeting of the American Nuclear Society
June 1-5, 2003
San Diego, CA



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Form 836 (8/00)

Testing of the ENDF66 Nuclear Data Library with MCNP™ Criticality Validation Suite

Russell D. Mosteller

Applied Physics Division, Los Alamos National Laboratory, Los Alamos, NM, 87545, mosteller@lanl.gov

INTRODUCTION

The ENDF66 nuclear data library¹ recently has been issued for use with the MCNP Monte Carlo code.² ENDF66 contains continuous-energy neutron interaction cross sections for 173 isotopes, based on release 6 of the 6th edition of the Evaluated Nuclear Data File (ENDF/B-VI.6).³ Furthermore, it contains probability tables for the treatment of resonances in the unresolved resonance region for 67 of those isotopes and delayed-neutron fission spectra for 22 of them.

Results have been obtained with ENDF66 for the cases in the MCNP criticality validation suite,⁴ and they have been compared with results obtained using a combination of the URES⁵ and ENDF60⁶ libraries. The URES library is derived from ENDF/B-VI.4 and contains data for 27 isotopes, while ENDF60 is based on ENDF/B-VI.2 and contains data for 122 isotopes. Neither URES nor ENDF60 contains delayed-neutron fission spectra. The URES library does contain probability tables for its constituent isotopes, but ENDF60 does not. Consequently, ENDF60 was used only for isotopes that are not present in URES. As a practical matter, very few of those isotopes were changed in going from ENDF/B-VI.4 to ENDF/B-VI.6, and those that did play only minor roles in the cases in the benchmark suite. Consequently, the results obtained with the combination of URES and ENDF60 can be considered representative of ENDF/B-VI.4.

CRITICALITY VALIDATION SUITE

The benchmarks employed in this study are summarized in Table I. In addition to the 26 cases from the criticality validation suite, four uranium cases with intermediate spectra — UH3 (6), Zeus (1), Zeus (3), and Zebra 8H — were included, because it became clear early on that significant reactivity differences would be observed for such cases. The specifications for all 30 cases are taken from the *International Handbook of Evaluated Criticality Benchmark Experiments*.⁷ All of the cases are at room temperature and pressure.

All the calculations were performed with MCNP4C2. All but one of the cases employed 1,250 generations of 5,000 neutron histories each, and the results from the first 50 generations were discarded. Consequently, the results reported for each of those cases are based on 6,000,000 active neutron histories. The one exception was Zebra 8H, which is extremely long running. That case employed 650 generations with the results from the first 50 generations being discarded. Consequently, the Zebra 8H results are based on 3,000,000 active histories.

RESULTS

The results from the 30 cases are presented in Table II. The only cases that show substantial differences in the ENDF66 and URES+ENDF60 results are the highly enriched uranium (HEU) cases with intermediate spectra, two of the intermediate-enriched-uranium (IEU) cases (BIG TEN and Zebra 8H), and Sheba II. The reductions in reactivity for the HEU cases with intermediate spectra are consistent with changes made in ENDF/B-VI.5 to the ²³⁵U cross sections in the intermediate-energy range. In contrast, the reactivity reductions for the two IEU cases and the reactivity increase for Sheba II are due to the inclusion of delayed-neutron spectra. In the two IEU cases, a significant fraction of the fissions occurs in ²³⁸U, which has an effective threshold for fission and a relatively large delayed-neutron fraction. The softer spectra of the delayed neutrons therefore lead to a slight reduction in the number of fissions and thereby to slightly lower reactivity. For Sheba II, the delayed-neutron spectra reduce neutron leakage and therefore increase reactivity slightly.

A closer look at the results indicates that reactivity increases slightly but significantly for the other thermal solution benchmarks and for Godiver, which has a significant thermal tail. These small increases are due primarily to the slight reduction in the 1/v portion of the radiative capture cross section for hydrogen that was made in ENDF/B-VI.5. That change returned that portion of cross section to its ENDF/B-V value.

TABLE I. MCNP Criticality Validation Suite and Additional Criticality Benchmarks

Fissile Fuel	Spectrum	Configuration	Case***	Benchmark k_{eff}
^{233}U	Fast	Bare sphere	Jezebel-233	1.0000 ± 0.0010
	Fast	Reflected by U	Flattop-23	1.0000 ± 0.0014
	Fast	Reflected by C	U233-MF-005 (2)	1.0000 ± 0.0030
	Intermediate	Solution	Falstaff (1)	1.0000 ± 0.0083
	Thermal	Solution	ORNL-11	1.0006 ± 0.0029
Highly Enriched Uranium	Fast	Bare sphere	Godiva	1.0000 ± 0.0010
	Fast	Reflected by U	Flattop-25	1.0000 ± 0.0030
	Fast	Reflected by H_2O	Godiver	0.9985 ± 0.0011
	Intermediate	Moderated by H, C	HISS/HUG	1.0000 ± 0.0040
	Intermediate	Moderated by H^*	UH_3 (6)	1.0000 ± 0.0047
	Intermediate	Moderated by C^{**}	Zeus (1)	0.9976 ± 0.0008
	Intermediate	Moderated by C^{**}	Zeus (2)	0.9997 ± 0.0008
	Intermediate	Moderated by C^{**}	Zeus (3)	1.0010 ± 0.0009
Thermal	3-D lattice in H_2O	HEU-MT-003 (4)	0.9876 ± 0.0040	
Thermal	Solution	ORNL-10	1.0015 ± 0.0026	
Intermediate-Enriched Uranium	Fast	Bare sphere	IEU-MF-003	1.0000 ± 0.0017
	Fast	Reflected by U	BIG TEN	0.9948 ± 0.0013
	Fast	Reflected by C	IEU-MF-004	1.0000 ± 0.0030
	Intermediate	Reflected by Steel	Zebra 8H	1.0300 ± 0.0025
Thermal	Lattice of pins in H_2O	IEU-CT-002 (3)	1.0017 ± 0.0044	
Low-Enriched Uranium	Thermal	PWR lattice in H_2O	BAW LRC XI (2)	1.0007 ± 0.0012
	Thermal	Solution	Sheba II	0.9991 ± 0.0029
Plutonium	Fast	Bare sphere	Jezebel	1.0000 ± 0.0020
	Fast	Bare sphere	Jezebel-240	1.0000 ± 0.0020
	Fast	Reflected by U	Flattop-Pu	1.0000 ± 0.0030
	Fast	Reflected by H_2O	Pu-MF-011	1.0000 ± 0.0010
	Fast	3-D lattice	Pu Buttons	1.0000 ± 0.0030
	Intermediate	Moderated by H, C	HISS/HPG	1.0000 ± 0.0110
	Thermal	MOX lattice	PNL-33	1.0024 ± 0.0021
	Thermal	Solution	PNL-2	1.0000 ± 0.0065

*Also reflected by depleted U

**Also reflected by Cu

***Numbers in parentheses indicate case number for benchmarks with more than one case

Although it is not immediately apparent from Table II, the inclusion of delayed-neutron spectra has a minor impact on the reactivity of several of the benchmarks. In general, they produce small negative changes for systems in which a significant fraction of the fissions occurs in a fertile isotope. Examples include the Flattop cases, which have normal uranium

reflectors, and Jezebel-240, which contains approximately 20 at.% ^{240}Pu . They also produce small positive reactivity changes for most fast and intermediate HEU systems. Changes are negligible for most thermal systems and for most plutonium and ^{233}U systems. This behavior is generally consistent with the conclusions from an earlier study.⁸

TABLE II. Results for Criticality Benchmarks

Case	k_{eff}		Δk^*	
	ENDF66	URES + ENDF60	ENDF66	URES + ENDF60
Jezebel-233	0.9928 ± 0.0002	0.9932 ± 0.0002	-0.0072 ± 0.0010	-0.0068 ± 0.0010
Flattop-23	1.0000 ± 0.0003	1.0008 ± 0.0003	0 ± 0.0014	0.0008 ± 0.0014
U233-MF-005 (2)	0.9972 ± 0.0003	0.9972 ± 0.0003	-0.0028 ± 0.0030	-0.0028 ± 0.0030
Falstaff (1)	0.9902 ± 0.0004	0.9897 ± 0.0004	-0.0098 ± 0.0083	-0.0103 ± 0.0083
ORNL-11	0.9969 ± 0.0002	0.9961 ± 0.0002	-0.0037 ± 0.0029	-0.0045 ± 0.0029
Godiva	0.9965 ± 0.0002	0.9966 ± 0.0002	-0.0035 ± 0.0010	-0.0034 ± 0.0010
Flattop-25	0.9968 ± 0.0003	0.9976 ± 0.0003	-0.0032 ± 0.0030	-0.0024 ± 0.0030
Godiver	0.9963 ± 0.0003	0.9953 ± 0.0003	-0.0022 ± 0.0011	-0.0032 ± 0.0011
HISS/HUG	1.0098 ± 0.0002	1.0125 ± 0.0002	0.0098 ± 0.0040	0.0125 ± 0.0040
UH ₃ (6)	0.9917 ± 0.0003	0.9934 ± 0.0003	-0.0083 ± 0.0047	-0.0066 ± 0.0047
Zeus (1)	0.9919 ± 0.0003	0.9942 ± 0.0003	-0.0057 ± 0.0009	-0.0034 ± 0.0009
Zeus (2)	0.9948 ± 0.0003	0.9977 ± 0.0003	-0.0049 ± 0.0009	-0.0020 ± 0.0009
Zeus (3)	0.9987 ± 0.0003	1.0016 ± 0.0003	-0.0023 ± 0.0009	0.0006 ± 0.0009
HEU-MT-003 (4)	0.9829 ± 0.0003	0.9827 ± 0.0003	-0.0037 ± 0.0040	-0.0039 ± 0.0040
ORNL-10	0.9986 ± 0.0002	0.9975 ± 0.0002	-0.0029 ± 0.0026	-0.0040 ± 0.0026
IEU-MF-003	0.9994 ± 0.0002	0.9997 ± 0.0003	-0.0006 ± 0.0017	-0.0003 ± 0.0017
BIG TEN	1.0073 ± 0.0002	1.0093 ± 0.0002	0.0125 ± 0.0013	0.0145 ± 0.0013
IEU-MF-004	1.0040 ± 0.0003	1.0041 ± 0.0003	0.0040 ± 0.0030	0.0041 ± 0.0030
Zebra 8H	1.0406 ± 0.0002	1.0426 ± 0.0002	0.0106 ± 0.0025	0.0126 ± 0.0025
IEU-CT-002 (3)	1.0010 ± 0.0003	1.0011 ± 0.0003	-0.0007 ± 0.0044	-0.0006 ± 0.0044
BAW LRC XI (2)	0.9977 ± 0.0003	0.9982 ± 0.0003	-0.0030 ± 0.0012	-0.0025 ± 0.0012
Sheba II	1.0107 ± 0.0003	1.0088 ± 0.0003	0.0126 ± 0.0029	0.0097 ± 0.0029
Jezebel	0.9976 ± 0.0002	0.9976 ± 0.0003	-0.0024 ± 0.0020	-0.0024 ± 0.0020
Jezebel-240	0.9978 ± 0.0002	0.9986 ± 0.0003	-0.0022 ± 0.0020	-0.0014 ± 0.0020
Flattop-Pu	1.0016 ± 0.0003	1.0026 ± 0.0003	0.0016 ± 0.0030	0.0026 ± 0.0030
Pu-MF-011	0.9974 ± 0.0003	0.9971 ± 0.0003	-0.0026 ± 0.0010	-0.0029 ± 0.0010
Pu Buttons	0.9962 ± 0.0003	0.9965 ± 0.0003	-0.0038 ± 0.0030	-0.0035 ± 0.0030
HISS/HPG	1.0105 ± 0.0002	1.0104 ± 0.0002	0.0105 ± 0.0110	0.0104 ± 0.0110
PNL-33	1.0038 ± 0.0003	1.0043 ± 0.0003	0.0014 ± 0.0021	0.0019 ± 0.0021
PNL-2	1.0018 ± 0.0004	1.0010 ± 0.0004	0.0018 ± 0.0065	0.0010 ± 0.0065

*Relative to benchmark k_{eff}

SUMMARY AND CONCLUSIONS

Based on the results from MCNP4C2 calculations with the MCNP Criticality Validation Suite and a few supplemental benchmarks, the ENDF66 library has been shown to produce mostly small changes in reactivity relative to the combina-

tion of the URES and ENDF60 libraries. However, larger changes do occur for HEU and IEU cases with intermediate spectra. The observed changes are consistent with the inclusion of delayed-neutron spectra and changes in the basic nuclear data between ENDF/B-VI.4 and ENDF/B-VI.6.

The most noticeable changes are for the HEU cases with intermediate spectra and for BIG TEN, Zebra 8H, and Sheba II. The changes degrade the agreement with the benchmark k_{eff} for all of the HEU cases with intermediate spectra except HISS/HUG. However, the reactivity bias for that case, and for BIG TEN, Zebra 8H, and Sheba II as well, still approaches or exceeds $0.01 \Delta k$.

REFERENCES

1. J. M. CAMPBELL, S. C. FRANKLE, R. 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 2002, p. 19, American Nuclear Society (2002).
2. "MCNP—A General Monte Carlo N-Particle Transport Code, Version 4C," LA-13709-M, J. F. BRIESMEISTER, ed., Los Alamos National Laboratory (March 2000).
3. "ENDF-102: Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6," BNL-NCS-44945-01/04-Rev., V. MCLANE, ed., Brookhaven National Laboratory (April 2001).
4. R. D. MOSTELLER, "Validation Suites for MCNP," *Proc. 12th Biennial Topl. Mtg. Radiation Protection and Shielding Div.*, Santa Fe, New Mexico, April 2002, p. 62, American Nuclear Society (2002).
5. R. C. LITTLE, R. E. MACFARLANE, "ENDF/B-VI Neutron Library for MCNP with Probability Tables," LA-UR-98-5718, Los Alamos National Laboratory (December 1998).
6. J. S. HENDRICKS, S. C. FRANKLE, J. D. COURT, "ENDF/B-VI Data for MCNP," LA-12891, Los Alamos National Laboratory (December 1994).
7. "International Handbook of Evaluated Criticality Safety Benchmark Experiments," NEA/NSC/DOC(95)03 (rev.), OECD-NEA (September 2002).
8. R. D. MOSTELLER, C. J. WERNER, "Reactivity Impact of Delayed Neutron Spectra on MCNP Calculations," *Trans. Am. Nucl. Soc.*, **82**, 235 (June 2000).