LA-UR-04-0123

Approved for public release; distribution is unlimited.

Title:	Comparison of ENDF/B-VI and Preliminary ENDF/B-VII Results for the MCNP [™] Criticality Validation Suite				
Author(s):	Russell D. Mosteller				
Submitted to:	2004 Annual Meeting of the American Nuclear Society June 13 - 17, 2004 Pittsburgh, PA				



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.

Comparison of ENDF/B-VI and Preliminary ENDF/B-VII Results for the MCNPTM Criticality Validation Suite

Russell D. Mosteller

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

An initial assessment of the impact of preliminary data proposed for ENDF/B-VII has been made using the MCNP criticality validation suite. Relative to ENDF/B-VI, the data changes primarily involve high-energy elastic and inelastic scattering in the uranium isotopes and ²³⁹Pu, as well as resonance parameters for ²³⁸U.

The criticality validation suite is a collection of 31 benchmarks taken from the *International Handbook of Evaluated Criticality Benchmark Experiments*.¹ It contains cases for a variety of fuels, including ²³³U, 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.

Three sets of calculations were performed for the suite using the MCNP5 Monte Carlo code.² The first set employed nuclear data from ENDF/B-VI Release 8, the final release for ENDF/B-VI. The second set employed preliminary ENDF/B-VII data generated by group T-16 at Los Alamos National Laboratory for the uranium isotopes and for ²³⁹Pu but retained ENDF/B-VI data for all other nuclides. The third set was the same as the second except that a new set of ²³⁸U resonance

parameters³ generated by researchers at Oak Ridge National Laboratory (ORNL) was used in combination with the T-16 evaluation.

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. The results from these calculations are presented in Table II.

The preliminary ENDF/B-VII data produce marked improvements in k_{eff} for bare spheres of ²³³U (Jezebel-233), HEU (Godiva), and plutonium (Jezebel and Jezebel-240) as well as the other unreflected HEU and plutonium cases (Tinkertoy02 (c-11) and Pu Buttons, respectively). Furthermore, the reactivity swings between those bare spheres and the corresponding Flattop cases (which enclose the sphere inside an annulus of normal uranium) are substantially decreased. The changes also significantly improve k_{eff} for BIG TEN, for HEU and plutonium spheres immersed in water (Godiver and Pu-MF-11, respectively), and for the thermal ²³³U solution

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 $(1)^{\dagger}$	SB-21/2	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

Table I. MCNP Criticality Validation Suite.

* Numbers in parentheses identify a specific case within a sequence of benchmarks

[†] Extrapolated to critical

 k_{∞} measurement

MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory

				Calculated k _{eff}		
Туре	Spectrum	Case	Benchmark k _{eff}	T-16 + ORNL ²³⁸ U	T-16	ENDF/B-VI
²³³ U	Fast	Jezebel-233 Flattop-23 U233-MF-05 (2)	$\begin{array}{c} 1.0000 \pm 0.0010 \\ 1.0000 \pm 0.0014 \\ 1.0000 \pm 0.0030 \end{array}$	$\begin{array}{c} 0.9984 \pm 0.0003 \\ 0.9988 \pm 0.0003 \\ 0.9964 \pm 0.0003 \end{array}$	$\begin{array}{c} 0.9989 \pm 0.0002 \\ 0.9985 \pm 0.0003 \\ 0.9968 \pm 0.0003 \end{array}$	$\begin{array}{c} 0.9931 \pm 0.0002 \\ 1.0003 \pm 0.0003 \\ 0.9976 \pm 0.0003 \end{array}$
	Intermediate	Falstaff (1)	1.0000 ± 0.0083	0.9876 ± 0.0005	0.9876 ± 0.0005	0.9894 ± 0.0005
	Thermal	SB-2½ ORNL-11	$\begin{array}{c} 1.0000 \pm 0.0024 \\ 1.0006 \pm 0.0029 \end{array}$	$\begin{array}{c} 0.9948 \pm 0.0005 \\ 1.0004 \pm 0.0002 \end{array}$	$\begin{array}{c} 0.9946 \pm 0.0005 \\ 1.0002 \pm 0.0002 \end{array}$	$\begin{array}{c} 0.9967 \pm 0.0005 \\ 0.9968 \pm 0.0002 \end{array}$
HEU	Fast	Godiva Tinkertoy-2 (c-11) Flattop-25 Godiver	$\begin{array}{c} 1.0000 \pm 0.0010 \\ 1.0000 \pm 0.0038 \\ 1.0000 \pm 0.0030 \\ 0.9985 \pm 0.0011 \end{array}$	$\begin{array}{c} 0.9992 \pm 0.0003 \\ 1.0001 \pm 0.0003 \\ 1.0025 \pm 0.0003 \\ 0.9978 \pm 0.0004 \end{array}$	$\begin{array}{c} 0.9990 \pm 0.0003 \\ 1.0001 \pm 0.0003 \\ 1.0023 \pm 0.0003 \\ 0.9969 \pm 0.0004 \end{array}$	$\begin{array}{c} 0.9962 \pm 0.0003 \\ 0.9972 \pm 0.0004 \\ 1.0024 \pm 0.0003 \\ 0.9948 \pm 0.0003 \end{array}$
	Intermediate	UH ₃ (6) Zeus (2)	$\begin{array}{c} 1.0000 \pm 0.0047 \\ 0.9997 \pm 0.0008 \end{array}$	$\begin{array}{c} 0.9926 \pm 0.0003 \\ 0.9948 \pm 0.0003 \end{array}$	$\begin{array}{c} 0.9925 \pm 0.0003 \\ 0.9945 \pm 0.0004 \end{array}$	$\begin{array}{c} 0.9914 \pm 0.0003 \\ 0.9942 \pm 0.0003 \end{array}$
	Thermal	SB-5 ORNL-10	$\begin{array}{c} 1.0015 \pm 0.0028 \\ 1.0015 \pm 0.0026 \end{array}$	$\begin{array}{c} 0.9943 \pm 0.0005 \\ 0.9994 \pm 0.0002 \end{array}$	$\begin{array}{c} 0.9941 \pm 0.0005 \\ 0.9986 \pm 0.0002 \end{array}$	$\begin{array}{c} 0.9963 \pm 0.0005 \\ 0.9992 \pm 0.0002 \end{array}$
IEU	Fast	IEU-MF-03 BIG TEN IEU-MF-04	$\begin{array}{c} 1.0000 \pm 0.0017 \\ 0.9948 \pm 0.0013 \\ 1.0000 \pm 0.0030 \end{array}$	$\begin{array}{c} 1.0026 \pm 0.0003 \\ 0.9950 \pm 0.0002 \\ 1.0077 \pm 0.0003 \end{array}$	$\begin{array}{c} 1.0032 \pm 0.0003 \\ 0.9953 \pm 0.0002 \\ 1.0081 \pm 0.0003 \end{array}$	$\begin{array}{c} 0.9987 \pm 0.0003 \\ 1.0071 \pm 0.0003 \\ 1.0038 \pm 0.0003 \end{array}$
	Intermediate	Zebra-8H	1.0300 ± 0.0025	1.0190 ± 0.0002	1.0197 ± 0.0003	1.0405 ± 0.0002
	Thermal	IEU-CT-02 (3) STACY-36	$\begin{array}{c} 1.0017 \pm 0.0044 \\ 0.9988 \pm 0.0013 \end{array}$	$\begin{array}{c} 1.0005 \pm 0.0003 \\ 0.9983 \pm 0.0003 \end{array}$	$\begin{array}{c} 0.9997 \pm 0.0003 \\ 0.9973 \pm 0.0003 \end{array}$	$\begin{array}{c} 1.0007 \pm 0.0003 \\ 0.9988 \pm 0.0003 \end{array}$
LEU	Thermal	BaW XI (2) LEU-ST-02 (2)	$\begin{array}{c} 1.0007 \pm 0.0012 \\ 0.9991 \pm 0.0029 \end{array}$	$\begin{array}{c} 0.9997 \pm 0.0003 \\ 0.9957 \pm 0.0003 \end{array}$	$\begin{array}{c} 0.9977 \pm 0.0003 \\ 0.9944 \pm 0.0003 \end{array}$	$\begin{array}{c} 0.9968 \pm 0.0003 \\ 0.9957 \pm 0.0003 \end{array}$
Pu	Fast	Jezebel Jezebel-240 Pu Buttons (3) Flattop-Pu THOR Pu-MF-11	$\begin{array}{l} 1.0000 \pm 0.0020 \\ 1.0000 \pm 0.0020 \\ 1.0000 \pm 0.0030 \\ 1.0000 \pm 0.0030 \\ 1.0000 \pm 0.0006 \\ 1.0000 \pm 0.0010 \end{array}$	$\begin{array}{c} 1.0004 \pm 0.0003 \\ 1.0001 \pm 0.0003 \\ 0.9986 \pm 0.0003 \\ 1.0006 \pm 0.0003 \\ 1.0081 \pm 0.0003 \\ 0.9986 \pm 0.0003 \end{array}$	$\begin{array}{l} 1.0004 \pm 0.0003 \\ 1.0001 \pm 0.0003 \\ 0.9986 \pm 0.0003 \\ 1.0008 \pm 0.0003 \\ 1.0081 \pm 0.0003 \\ 0.9986 \pm 0.0003 \end{array}$	$\begin{array}{c} 0.9975 \pm 0.0003 \\ 0.9979 \pm 0.0003 \\ 0.9962 \pm 0.0003 \\ 1.0013 \pm 0.0003 \\ 1.0062 \pm 0.0003 \\ 0.9970 \pm 0.0003 \end{array}$
	Intermediate	HISS/HPG	1.0000 ± 0.0110	1.0111 ± 0.0005	1.0111 ± 0.0005	1.0104 ± 0.0003
	Thermal	PNL-33 PNL-2	$\begin{array}{c} 1.0024 \pm 0.0021 \\ 1.0000 \pm 0.0065 \end{array}$	$\begin{array}{c} 1.0057 \pm 0.0003 \\ 1.0039 \pm 0.0010 \end{array}$	$\begin{array}{c} 1.0053 \pm 0.0007 \\ 1.0039 \pm 0.0010 \end{array}$	$\begin{array}{c} 1.0029 \pm 0.0003 \\ 1.0033 \pm 0.0005 \end{array}$

Table II MCNP5 Results for Criticality Safety Validation Set.

(ORNL-11). In addition, inclusion of the ORNL resonance parameters for ²³⁸U produces a significantly better value for k_{eff} for the HEU sphere immersed in water (Godiver) and for the lattice of LEU fuel pins in water (B&W XI (2)). Furthermore, relative to the T-16 results, the ORNL resonance parameters improve k_{eff} for the thermal HEU, IEU, and LEU solutions (ORNL-10, STACY-36, and LEU-ST-02 (2), respectively).

At the same time, the preliminary ENDF/B-VII data produce worse results than ENDF/B-VI for

thermal lattices of ²³³U and HEU pins in water (SB-2¹/₂ and SB-5, respectively), for the bare IEU sphere (IEU-MF-03) and the IEU sphere reflected by graphite (IEU-MF-04), for the plutonium sphere reflected by thorium (THOR), and for the MOX lattice in water (PNL-33). Furthermore, k_{eff} for the uranium cases with intermediate spectra remains substantially underpredicted, while k_{eff} for the plutonium case with an intermediate spectrum (HISS/HPG) continues to be significantly over-predicted.

In conclusion, preliminary ENDF/B-VII data for the uranium isotopes and ²³⁹Pu produce improvements for most of the cases with fast spectra, BIG TEN, and the lattice of LEU fuel pins in water. However, improvements still are needed in some areas, particularly those cases with intermediate spectra.

REFERENCES

- 1. International Handbook of Evaluated Criticality Safety Benchmark Experiments, OECD Nuclear Energy Agency report NEA/NSC/DOC(95)03, September 2003 Edition.
- 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 Lab. (April 2003).
- H. DERRIEN, L. C. LEAL, N. M. LARSON, "New Evaluation of ²³⁸U Neutron Resonance Parameters," *Proc.* 7th Int. Conf. Nuclear Criticality Safety (ICNC2003), Tokai, Ibaraki, Japan (October 2003).