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ENDF/B-VI and Preliminary ENDF/B-VII Results for the MCNP Criticality Validation Suite

Author(s):

Russell D. Mosteller
Robert C. Little

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Russell D. Mosteller
Robert C. Little

Los Alamos National Laboratory, P. O. Box 1663, Los Alamos, NM 87545 USA

To Be Presented at the 2004 Annual Meeting of the
Cross Section Evaluation Working Group
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The MCNP Criticality Validation Suite is a collection of 31 benchmarks taken from the *International Handbook of Evaluated Criticality Benchmark Experiments*. It includes cases with a variety of fuels, moderators, reflectors, spectra, and geometries. Specifically, it contains six cases with ^{233}U fuel, eight cases with highly enriched uranium (HEU), six cases with intermediate-enriched uranium (IEU), two cases with low-enriched uranium (LEU), and nine cases with plutonium. Except for LEU (which can reach criticality only with a thermal spectrum), there are cases with fast, intermediate, and thermal spectra for each of these fuels. The fast cases include bare spheres, cores with heavy reflectors, cores with light reflectors, and lattices. The thermal cases include lattices of fuel pins and solutions for each of the five types of fuel. The cases with intermediate spectra are less uniform, due to the limited number of experiments with such spectra.

Two sets of MCNP5 calculations were performed for the MCNP Criticality Validation Suite. 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 ^{237}Np, the uranium isotopes, and ^{239}Pu along with new sets of resonance parameters for ^{233}U, ^{235}U, and ^{238}U generated by researchers at Oak Ridge National Laboratory.

The preliminary ENDF/B-VII data produce marked improvement in k_{eff} for bare spheres of ^{233}U , HEU, and plutonium. Furthermore, the reactivity swings between those cases and corresponding cases that enclose the sphere inside an annulus of normal uranium are substantially decreased. They also significantly improve k_{eff} for a cylinder of IEU reflected by normal uranium, for HEU and plutonium spheres immersed in water, and for a lattice of LEU fuel pins in water.

At the same time, they produce worse results than ENDF/B-VI for thermal lattices of ^{233}U and HEU pins, for an IEU sphere reflected by graphite, and for a plutonium sphere reflected by thorium. Furthermore, k_{eff} for uranium cases with intermediate spectra remain substantially underpredicted, while k_{eff} for a plutonium case with an intermediate spectrum continues to be significantly overpredicted.

AMERICAN NUCLEAR SOCIETY SPECIAL SESSION

CSEWG and Nuclear Data: The Legacy of Sol Pearlstein

This session is dedicated to Sol Pearlstein, who for many years was the director of the National Nuclear Data Center at Brookhaven National Laboratory and the moving force behind the Cross Section Evaluation Working Group. Under Sol's leadership, the accuracy of ENDF/B data was improved considerably, and the content of the ENDF/B files was substantially expanded. In addition, he was the author of a number of journal articles and many technical reports in the area of nuclear data methodology.

This session will include an opening memorial by a Charles Dunford, a friend and close colleague of Sol's. The remaining papers will be technical in nature:

> Charles L. Dunford, "Personal Reminiscences of Sol Pearlstein"
>
> J. J. Wagschal and Y. Yeivin, "When Even Pearlstein the Purist Engaged in Adjustment"
>
> Luiz Leal and Herve Derrien, "Statistical Properties of the s- and p-Wave Resonances of ^{238}U"
>
> S. C. Frankle and J. M. Harp, "Tritium Production in $^{6,7}Li$ from 14-MeV Neutrons"
>
> T. Zhou, A. I. Hawari, B. W. Wehring, V. H. Gillette, and I. I. Al-Qasir, "Benchmark for Beryllium Thermal Neutron Scattering Cross Sections"
>
> A. C. Kahler, "Cross Section Testing with HEU and LEU Thermal Solution ICSBEP Benchmarks"
>
> David Loaiza, Rene Sanchez, and David Hayes, "Sensitivity Analysis for the Np-237 and HEU Fast System Reflected by Low Carbon Steel"
>
> Russell D. Mosteller, Peter J. Jaegers, and Roger W. Brewer, "Analysis of the Fourth Zeus Critical Experiment"

The session will be held on the afternoon of Monday, November 15, during the annual meeting of the American Nuclear Society in Washington, DC. This session is sponsored by the Reactor Physics Division and is co-sponsored by the Radiation Protection and Shielding Division and the Nuclear Criticality Safety Division.

ENDF/B-VI and Preliminary ENDF/B-VII Results for the MCNP Criticality Validation Suite

Russell D. Mosteller
Robert C. Little

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

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OVERVIEW OF PRESENTATION

Succinct Description of MCNP Criticality Validation Suite

Characteristics of Preliminary Nuclear Data for ENDF/B-VII

Comparison of Results from MCNP5 Using Final ENDF/B-VI and Preliminary ENDF/B-VII Nuclear Data Libraries

Some Remaining Areas for Improvement

Conclusions

MCNP Criticality Validation Suite

Cases were selected to encompass a wide variety of

Fissile isotopes	:	^{233}U, ^{235}U, and ^{239}Pu
Spectra	:	Fast, intermediate, and thermal
Compositions	:	Metals, oxides, and solutions
Configurations	:	Bare and reflected spheres and cylinders, 2-D and 3-D lattices, and infinite homogeneous and heterogeneous regions

^{235}U Cases were subdivided into HEU, IEU, AND LEU

Input specifications for all 31 cases are taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*

CASES IN THE MCNP CRITICALITY VALIDATION SUITE

Fuel	Fast			Intermed	Thermal	
	Bare	Heavy Reflector	Light Reflector	Various	Lattice of Fuel Pins	Solution
^{233}U	Jezebel-233	Flattop-23	U233-MF-05	Falstaff (1)*	SB-2½	ORNL-11
HEU	Godiva Tinkertoy-2 (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 (2)	STACY (36)
LEU					B&W XI (2)	LEU-ST-02 (2)
Pu	Jezebel Jezebel-240 Pu Buttons (103)	Flattop-Pu THOR	Pu-MF-11	HISS/HPG†	PNL-33	PNL-2

* Extrapolated to critical   † k_∞ measurement

CASES IN THE MCNP CRITICALITY VALIDATION SUITE (Cont'd)

All cases with heavy reflectors use normal uranium except THOR, which uses thorium

Light reflectors are beryllium for U233-MF-05, graphite for IEU-MF-04, and water for Godiver and Pu-MF-11

All lattices of fuel pins are in water

SB-5 includes an outer blanket of ThO_2 pins

All solutions are in water

All solutions are nitrates except LEU-ST-02 (2), which is uranyl fluoride

PURPOSE AND USE OF THE MCNP CRITICALITY VALIDATION SUITE

The MCNP Criticality Validation Suite was developed to assess the reactivity impact of future improvements to MCNP as well as changes to its associated nuclear data libraries

Suite is *not* an absolute indicator of the accuracy or reliability of a given nuclear data library, nor is it intended to be

Suite can provide a general indication of the overall performance of a nuclear data library

Suite can provide an early warning of unexpected or unintended consequences resulting from changes to nuclear data

PRELIMINARY NUCLEAR DATA FOR ENDF/B-VII

Final version of ENDF/B-VI (Release 8) was released in October 2001

Are future nuclear data libraries likely to produce improved results?

Preliminary changes to ^{237}Np, ^{233}U, ^{234}U ^{235}U, ^{236}U, ^{238}U, and ^{239}Pu for ENDF/B-VII offer encouragement

Data changes primarily involve high-energy fission cross sections, $\bar{\nu}$, elastic and inelastic scattering, fission spectra, and delayed neutrons (LANL group T-16), in conjunction with revised resonance parameters for ^{233}U, ^{235}U, and ^{238}U (ORNL)

Recently released T16_2003 nuclear data library contains LANL T-16 nuclear data for ^{237}Np, uranium isotopes, ^{239}Pu, and a few other nuclides (but not ORNL resonance parameters for ^{233}U, ^{235}U, or ^{238}U)

MCNP5 CALCULATIONS FOR CRITICALITY VALIDATION SUITE

All calculations were performed with continuous-energy nuclear data libraries

ENDF/B-VI calculations employed the ACTI and ENDF66 nuclear data libraries and the SAB2002 library of thermal scattering laws

Preliminary ENDF/B-VII calculations employed the T16_2003 nuclear data library augmented by the ORNL resonance parameters for ^{233}U, ^{235}U, and ^{238}U but retained ENDF/B-VI nuclear data for all other nuclides

Each calculation employed 550 generations with 10,000 neutrons per generation (SB-5 and Zebra-8H employed 350 generations)

Results from first 50 generations were excluded from the statistics

Results therefore are based on 5,000,000 active histories for each case (3,000,000 for SB-5 and Zebra-8H)

RESULTS FOR ^{233}U BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}	
		Pre-ENDF/B-VII	ENDF/B-VI
Jezebel-233	1.0000 ± 0.0010	0.9988 ± 0.0003	0.9931 ± 0.0003
Flattop-23	1.0000 ± 0.0014	0.9987 ± 0.0003	1.0003 ± 0.0003
U233-MF-05	1.0000 ± 0.0030	0.9967 ± 0.0003	0.9976 ± 0.0003
Falstaff (1)	1.0000 ± 0.0083	0.9876 ± 0.0005	0.9894 ± 0.0005
SB-2½	1.0000 ± 0.0024	0.9948 ± 0.0004	0.9967 ± 0.0005
ORNL-11	1.0006 ± 0.0029	1.0000 ± 0.0002	0.9968 ± 0.0002

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

k_{eff} for Jezebel-233 improves dramatically, and reactivity swing from Jezebel-233 to Flattop-23 is eliminated

k_{eff} for ORNL-11 improves substantially, although results deteriorate for U233-MF-05 and SB-2½

RESULTS FOR HEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}	
		Pre-ENDF/B-VII	ENDF/B-VI
Godiva	1.0000 ± 0.0010	0.9993 ± 0.0003	0.9962 ± 0.0003
Tinkertoy-2 (11)	1.0000 ± 0.0038	1.0004 ± 0.0003	0.9972 ± 0.0003
Flattop-25	1.0000 ± 0.0030	1.0030 ± 0.0003	1.0024 ± 0.0003
Godiver	0.9985 ± 0.0011	0.9975 ± 0.0003	0.9948 ± 0.0003
UH_3 (6)	1.0000 ± 0.0047	0.9953 ± 0.0004	0.9914 ± 0.0003
Zeus (2)	0.9997 ± 0.0008	0.9976 ± 0.0003	0.9942 ± 0.0003
SB-5	1.0015 ± 0.0028	0.9960 ± 0.0006	0.9963 ± 0.0005
ORNL-10	1.0015 ± 0.0026	0.9991 ± 0.0002	0.9992 ± 0.0002

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

k_{eff} improves substantially for Godiva, Godiver, UH_3 (6) and Zeus (2)

Reactivity swing from Godiva to Flattop-25 is reduced significantly

RESULTS FOR IEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}	
		Pre-ENDF/B-VII	ENDF/B-VI
IEU-MF-03	1.0000 ± 0.0017	1.0028 ± 0.0003	0.9987 ± 0.0003
BIG TEN	0.9948 ± 0.0013	0.9941 ± 0.0002	1.0071 ± 0.0002
IEU-MF-04	1.0000 ± 0.0030	1.0078 ± 0.0003	1.0038 ± 0.0003
Zebra-8H	1.0300 ± 0.0025	1.0188 ± 0.0002	1.0405 ± 0.0002
IEU-CT-02 (2)	1.0017 ± 0.0044	1.0009 ± 0.0003	1.0007 ± 0.0003
STACY (36)	0.9988 ± 0.0013	0.9988 ± 0.0003	0.9988 ± 0.0003

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

k_{eff} improves dramatically for BIG TEN

k_{eff} is worse for IEU-MF-03 and IEU-MF-04 and drops substantially for Zebra-8H

For IEU-CT-02 (2) and STACY (36), changes to resonance parameters for ^{235}U and ^{238}U offset reactivity effects of scattering changes for uranium isotopes

RESULTS FOR LEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}	
		Pre-ENDF/B-VII	ENDF/B-VI
B&W XI (2)	1.0007 ± 0.0012	1.0000 ± 0.0003	0.9968 ± 0.0003
LEU-ST-02 (2)	1.0024 ± 0.0037	0.9967 ± 0.0003	0.9957 ± 0.0003

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

k_{eff} improves substantially for B&W XI (2), which eliminates need for *ad hoc* adjustment to ^{238}U resonance integral (used in many nuclear data libraries since early 1970s)

For LEU-ST-02 (2), changes to resonance parameters for ^{235}U and ^{238}U offset reactivity effects of scattering changes for uranium isotopes

RESULTS FOR PU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}	
		Pre-ENDF/B-VII	ENDF/B-VI
Jezebel	1.0000 ± 0.0020	1.0004 ± 0.0003	0.9975 ± 0.0003
Jezebel-240	1.0000 ± 0.0020	1.0001 ± 0.0003	0.9979 ± 0.0003
Pu Buttons (103)	1.0000 ± 0.0030	0.9986 ± 0.0003	0.9962 ± 0.0003
Flattop-Pu	1.0000 ± 0.0030	1.0006 ± 0.0003	1.0019 ± 0.0003
THOR	1.0000 ± 0.0006	1.0081 ± 0.0003	1.0062 ± 0.0003
Pu-MF-11	1.0000 ± 0.0010	0.9986 ± 0.0003	0.9970 ± 0.0003
HISS/HPG	1.0000 ± 0.0110	1.0111 ± 0.0003	1.0105 ± 0.0003
PNL-33	1.0024 ± 0.0021	1.0066 ± 0.0003	1.0029 ± 0.0003
PNL-2	1.0000 ± 0.0065	1.0039 ± 0.0005	1.0033 ± 0.0005

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

Results are as good or better for all fast cases except THOR, and reactivity swing from Jezebel to Flattop-Pu is eliminated

k_{eff} RATIOS FOR BARE SPHERES AND CORRESPONDING U-REFLECTED CASES

Cases		$(k_{eff})_{Sphere}$ / $(k_{eff})_{U\text{-}Refl}$		
Bare Sphere	U-Reflected	Benchmark	Pre-ENDF/B-VII	ENDF/B-VI
Jezebel-233	Flattop-23	1.0000 ± 0.0017	1.0001 ± 0.0004	0.9928 ± 0.0004
Godiva	Flattop-25	1.0000 ± 0.0032	0.9963 ± 0.0004	0.9938 ± 0.0004
IEU-MF-03	BIG TEN	1.0052 ± 0.0021	1.0088 ± 0.0004	0.9917 ± 0.0004
Jezebel	Flattop-Pu	1.0000 ± 0.0036	0.9998 ± 0.0004	0.9956 ± 0.0004

$\sigma < |\Delta \text{Ratio}| \leq 2\sigma$ $|\Delta \text{Ratio}| > 2\sigma$

Pre-ENDF/B-VII ratios increase and show improvement for all four cases relative to ENDF/B-VI

Difference in Pre-ENDF/B-VII ratio exceeds 1σ for HEU, even though differences in component values for k_{eff} do not

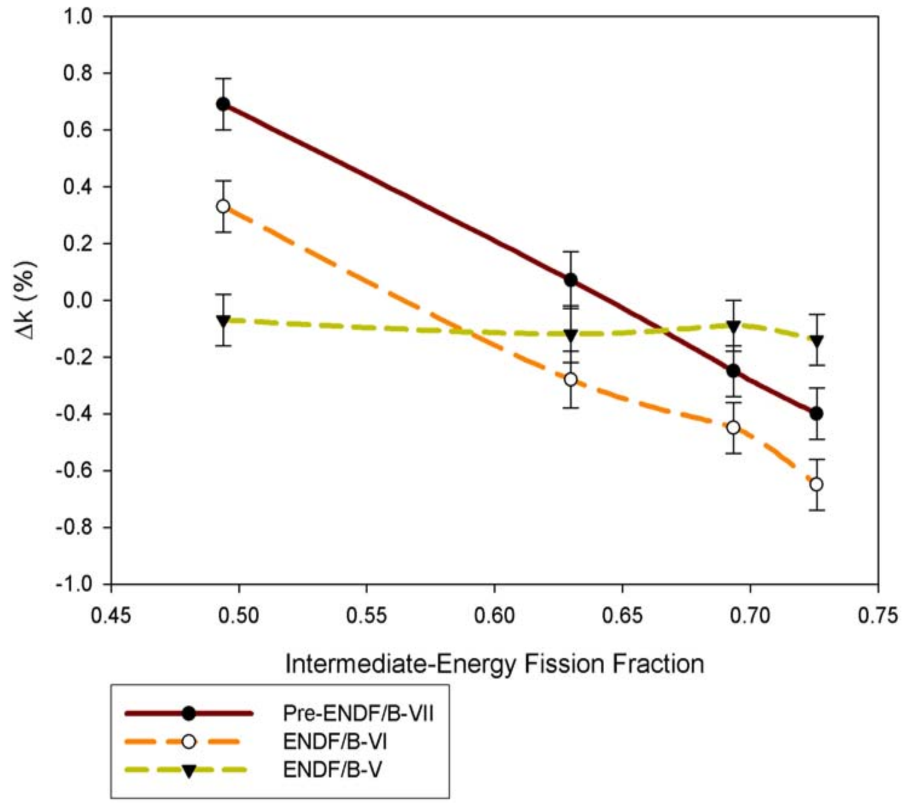
SUMMARY OF RESULTS FOR MCNP CRITICALITY VALIDATION SUITE

Range	Pre-ENDF/B-VII	ENDF/B-VI
$\|\Delta k\| \leq \sigma$	18	13
$\sigma < \|\Delta k\| \leq 2\sigma$	8	9
$\|\Delta k\| > 2\sigma$	5	9

Substantial improvements for bare metal spheres (Jezebel-233, Godiva, and Jezebel), BIG TEN, HEU and Pu metal spheres in water (Godiver and Pu-MF-011, respectively), and LEU lattice (B&W XI (2))

ORNL resonance parameters improve results for Godiver, ORNL-10, IEU-CT-03, STACY (36), B&W XI (2), and LEU-ST-02 (2)

RESULTS FOR ZEUS HEU-GRAPHITE BENCHMARKS



Calculated values for k_{eff} from both ENDF/B-VI and Pre-ENDF/B-VII exhibit an energy-dependent bias

RESULTS FOR NEPTUNIUM SPHERE BENCHMARK

k_{eff}		
Benchmark	Pre-ENDF/B-VII	ENDF/B-VI
1.0019 ± 0.0036	0.9922 ± 0.0003	0.9889 ± 0.0002

$|\Delta k| > 2\sigma$

Pre-ENDF/B-VII result is better than the ENDF/B-VI result, but it still is substantially lower (~ 1% Δk) than the benchmark value

Caveat: calculated results for a similar experiment with a plutonium sphere also show a large reactivity discrepancy, in contradiction to other benchmarks with plutonium reflected by HEU

RESULTS FOR HEAVY-WATER BENCHMARKS

Series	Case	Benchmark k_{eff}	Calculated k_{eff}		
			Pre-ENDF/B-VII + ENDF/B-VI.0 ^{2}H	Pre-ENDF/B-VII	ENDF/B-VI
Reflected Spheres (HEU-SOL-THERM-004)	1	1.0000 ± 0.0033	0.9948 ± 0.0004	0.9902 ± 0.0004	0.9839 ± 0.0004
	2	1.0000 ± 0.0036	0.9902 ± 0.0004	0.9846 ± 0.0004	0.9798 ± 0.0004
	3	1.0000 ± 0.0039	0.9962 ± 0.0004	0.9908 ± 0.0004	0.9861 ± 0.0004
	4	1.0000 ± 0.0046	0.9984 ± 0.0004	0.9937 ± 0.0005	0.9886 ± 0.0004
	5	1.0000 ± 0.0052	0.9969 ± 0.0004	0.9912 ± 0.0004	0.9871 ± 0.0004
	6	1.0000 ± 0.0059	0.9931 ± 0.0005	0.9876 ± 0.0004	0.9837 ± 0.0004
Unreflected Cylinders (HEU-SOL-THERM-020)	1	0.9966 ± 0.0116	1.0023 ± 0.0005	0.9902 ± 0.0005	0.9918 ± 0.0005
	2	0.9956 ± 0.0093	1.0079 ± 0.0005	0.9966 ± 0.0005	0.9967 ± 0.0005
	3	0.9957 ± 0.0079	1.0150 ± 0.0005	1.0046 ± 0.0005	1.0055 ± 0.0005
	4	0.9955 ± 0.0078	1.0136 ± 0.0005	1.0034 ± 0.0005	1.0029 ± 0.0005
	5	0.9959 ± 0.0077	1.0194 ± 0.0005	1.0114 ± 0.0005	1.0114 ± 0.0005

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

RESULTS FOR HEAVY-WATER BENCHMARKS (Continued)

Benchmarks all have large standard deviations

Biases for HEU-SOL-THERM-020 benchmarks are due entirely to *calculated* omission of room return

Differences between ENDF/B-VII results with ENDF/B-VI ^{2}H and ENDF/B-VI.2 ^{2}H are primarily due to angular scattering in the MeV range, even though these cases have thermal or intermediate spectra

Differences between the two evaluations for ^{2}H should be reviewed and, if possible, reconciled before the initial version of ENDF/B-VII is issued

RESULTS FOR 48-INCH SPHERE OF PLUTONIUM NITRATE IN WATER

k_{eff}		
Benchmark	Pre-ENDF/B-VII	ENDF/B-VI
1.0003 ± 0.0003	1.0193 ± 0.0002	1.0189 ± 0.0002

$|\Delta k| > 2\sigma$

Sphere is same one used for ORNL-10 and ORNL-11

Very thermal spectrum, with very little leakage

CONCLUSIONS

Overall, Pre-ENDF/B-VII data produce major improvements in reactivity relative to ENDF/B-VI

Reactivity swings from bare metal spheres to corresponding systems reflected by normal uranium are eliminated or substantially reduced

Need for *ad hoc* adjustment to ^{238}U resonance integral may be eliminated

Improvements still are needed, particularly for cases with

- intermediate spectra
- plutonium in thermal spectra
- thorium
- deuterium
- neptunium (probably)