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Title: Comparison of Results from the MCNP Criticality Validation Suite Using ENDF/B-VI and Preliminary ENDF/B-VII Nuclear Data

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Comparison of Results from the MCNP Criticality Validation Suite Using ENDF/B-VI and Preliminary ENDF/B-VII Nuclear Data

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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 U-233 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.

Three sets of MCNP5 calculations were performed for the MCNP Criticality Validation Suite. The first set employed nuclear data derived from ENDF/B-V, while the second set employed nuclear data from ENDF/B-VI Release 8, the final release for ENDF/B-VI. The third set employed preliminary ENDF/B-VII data generated by group T-16 at Los Alamos National Laboratory for the uranium isotopes and for plutonium-239 along with new sets of resonance parameters for ^{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 (Jezebel). 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.

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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

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

* Extrapolated to critical † k_∞ measurement

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 ^{233}U, ^{235}U, ^{236}U, ^{238}U, and ^{239}Pu for ENDF/B-VII offer encouragement

Data changes primarily involve high-energy elastic and inelastic scattering in the uranium isotopes and ^{239}Pu (LANL group T-16), as well as resonance parameters for ^{235}U and ^{238}U (ORNL)

MCNP5 CALCULATIONS FOR CRITICALITY VALIDATION SUITE

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	0.9992 ± 0.0002	0.9931 ± 0.0003
Flattop-23	1.0000 ± 0.0014	0.9986 ± 0.0003	1.0003 ± 0.0003
U233-MF-05	1.0000 ± 0.0030	0.9966 ± 0.0003	0.9976 ± 0.0003
Falstaff-1	1.0000 ± 0.0083	0.9877 ± 0.0005	0.9894 ± 0.0005
SB-2½	1.0000 ± 0.0024	0.9948 ± 0.0005	0.9967 ± 0.0005
ORNL-11	1.0006 ± 0.0029	1.0005 ± 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	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	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

k_{eff} improves substantially for Godiva, Godiver, UH_3 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	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

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 and STACY-36, changes to ^{238}U resonance parameters 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	1.0024 ± 0.0037	0.9967 ± 0.0003	0.9957 ± 0.0003

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, changes to ^{238}U resonance parameters 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	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

Striking improvement in k_{eff} for fast cases except THOR, and reactivity swing from Jezebel to Flattop-Pu is eliminated

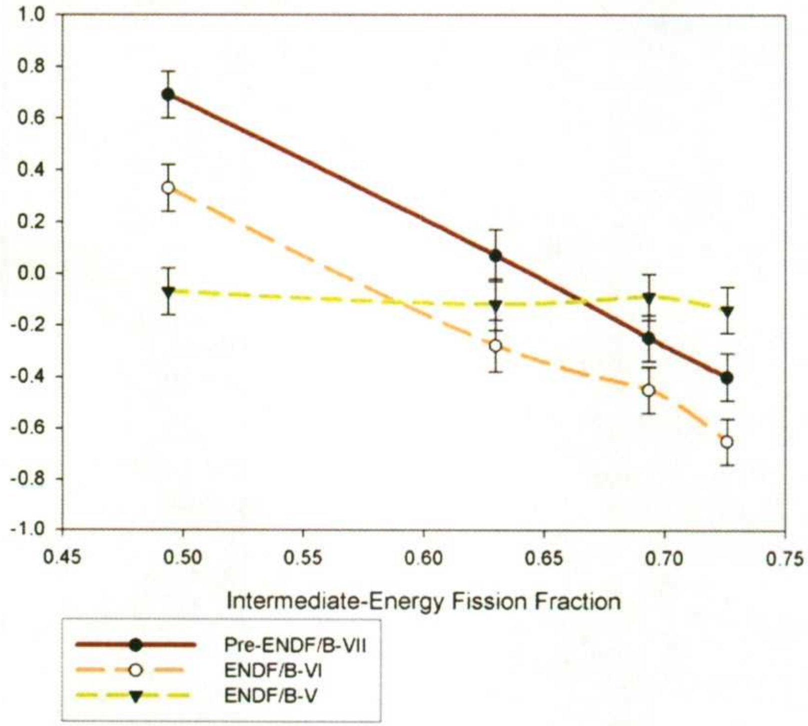
SUMMARY OF RESULTS FOR MCNP CRITICALITY VALIDATION SUITE

Range	Pre-ENDF/B-VII	ENDF/B-VI
$\lvert\Delta k\rvert \leq \sigma$	19	13
$\sigma < \lvert\Delta k\rvert \leq 2\sigma$	7	9
$\lvert\Delta k\rvert > 2\sigma$	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

RESULTS FOR ZEUS HEU-GRAPHITE BENCHMARKS



ENDF/B-VI and Pre-ENDF/B-VII results show an energy-dependent bias

RESULTS FOR HEAVY-WATER BENCHMARKS

Series	Case	Benchmark k_{eff}	Calculated k_{eff}		
			Pre-ENDF/B-VII + ENDF/B-VI.0 ^{2}D	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

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

Pre-ENDF/B-VII result is better than the ENDF/B-VI result, but it still is substantially lower than the benchmark value

CONCLUSIONS

Overall, Pre-ENDF/B-VII produces major reactivity improvements relative to ENDF/B-VI

Reactivity swings from bare spheres to similar 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, thorium, deuterium, or neptunium