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An Assessment of ENDF/B-VI Releases Using the MCNP™ Criticality Validation Suite

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The final release of version VI of the Evaluated Nuclear Data File, release 8, was distributed in October 2001. That release came approximately two decades after the final release of its predecessor, ENDF/B-V. In the interim, several intermediate releases of ENDF/B-VI incorporated substantive changes to nuclear data for a large number of isotopes. This study provides an assessment of reactivity behavior produced by the nuclear data in that final release and in three of the preceding intermediate releases, using the MCNP5 Monte Carlo code and the benchmarks in the MCNP criticality validation suite.

Relative to the second interim release, the final release produces little, if any, net improvement. Results improve for some cases but deteriorate for others. Clearly, data changes that improve results for some cases degrade them for others. In addition, poor agreement with the benchmark values for certain cases remains essentially unaffected.

Collectively, the results obtained suggest that the cross sections for a number of nuclides still need improvement. Adjustments to the cross sections for ^{232}Th, ^{233}U, ^{235}U, ^{238}U, and ^{239}Pu conceivably could produce better agreement with the benchmark values of k_{eff} for several of the cases in the suite. Improvements might also result from returning to cross sections from earlier interim releases for certain nuclides.

AN ASSESSMENT OF ENDF/B-VI RELEASES USING THE MCNP™ CRITICALITY VALIDATION SUITE

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OVERVIEW OF PRESENTATION

Background

Succinct Description of MCNP Criticality Validation Suite

ENDF/B-VI Nuclear Data Libraries

Calculated Results for Interim and Final ENDF/B-VI Releases

Comparison of Results Using ENDF/B-V and Final ENDF/B-VI Libraries

Conclusions

BACKGROUND

Final Release of ENDF/B-VI Occurred in October 2001, Nearly Two Decades after Final Release of ENDF/B-V

Subsequent to the Pre-Release Version (ENDF/B-VI.0), ENDF/B-VI Had 8 Interim Releases, ENDF/B-VI.1 through ENDF/B-VI.8

This Study Assesses the Changes in Reactivity Behavior for 4 of Those Releases Using the MCNP Criticality Validation Suite:

ENDF/B-VI.2
ENDF/B-VI.4
ENDF/B-VI.6
ENDF/B-VI.8 (Final)

MCNP CRITICALITY VALIDATION SUITE

MCNP Criticality Validation Suite Was Developed to Assess Reactivity Impact of Future Improvements to MCNP as Well as Changes to Its Associated Nuclear Data Libraries

Suite Contains 31 Benchmarks, All Taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*

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

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-003	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

MCNP NUCLEAR DATA LIBRARIES

Library	Issued	Source	Total Nuclides	Nuclides with Probability Tables for Unresolved Resonance Region	Fissioning Nuclides with Delayed-Neutron Spectra
ENDF60	1994	ENDF/B-VI.2	122	0	0
URES	1998	ENDF/B-VI.4	27	27	0
ENDF66	2002	ENDF/B-VI.6	173	67	22
ACTI	2002	ENDF/B-VI.8	41	4	0

SAB2002, a Library of Thermal Scattering Laws S(α,β), Was Released in 2002

Smaller Libraries Can Be Combined with Previous Libraries to Produce Sets of Nuclear Data Corresponding to Specific ENDF/B-VI Releases

(e.g., URES + ENDF60 $\cong$ ENDF/B-VI.4)

MCNP5 CALCULATIONS

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)

Calculations with ENDF66 and/or ACTI Libraries Used SAB2002 as Well

RESULTS FOR ^{233}U BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}			
		VI.8	VI.6	VI.4	VI.2
Jezebel-233	1.0000±0.0010	0.9931±0.0002	0.9931±0.0002	0.9932±0.0003	0.9928±0.0003
Flattop-23	1.0000±0.0014	1.0003±0.0003	1.0003±0.0003	1.0009±0.0003	1.0008±0.0003
U233-MF-05	1.0000±0.0030	0.9976±0.0003	0.9963±0.0005	0.9965±0.0003	0.9971±0.0003
Falstaff-1	1.0000±0.0083	0.9894±0.0005	0.9902±0.0005	0.9889±0.0005	0.9890±0.0005
SB-2½	1.0000±0.0024	0.9967±0.0005	0.9974±0.0005	0.9959±0.0005	0.9978±0.0005
ORNL-11	1.0006±0.0029	0.9968±0.0002	0.9974±0.0002	0.9952±0.0002	0.9956±0.0002

$1\sigma < \Delta k \leq 2\sigma$ $\Delta k > 2\sigma$

ENDF/B-VI Cross Sections for ^{233}U Did Not Change

Reactivity Changes Are Due to Other Isotopes (H, Be, N, O, Etc.)

RESULTS FOR HEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}			
		VI.8	VI.6	VI.4	VI.2
Godiva	1.0000±0.0010	0.9962±0.0003	0.9962±0.0003	0.9967±0.0003	0.9965±0.0003
Tinkertoy-2	1.0000±0.0038	0.9972±0.0003	0.9972±0.0003	0.9981±0.0003	0.9987±0.0003
Flattop-25	1.0000±0.0030	1.0024±0.0003	1.0024±0.0005	1.0022±0.0003	1.0027±0.0003
Godiver	0.9985±0.0011	0.9948±0.0003	0.9954±0.0004	0.9955±0.0004	0.9970±0.0003
UH_3	1.0000±0.0047	0.9914±0.0003	0.9915±0.0003	0.9928±0.0004	1.0080±0.0004
Zeus-2	0.9997±0.0008	0.9942±0.0003	0.9941±0.0003	0.9977±0.0003	1.0088±0.0004
SB-5	1.0015±0.0028	0.9963±0.0005	0.9980±0.0005	0.9951±0.0005	0.9972±0.0005
ORNL-10	1.0015±0.0026	0.9992±0.0002	0.9990±0.0002	0.9970±0.0002	0.9970±0.0002

Results for ORNL-10 Improve Because of Changes to H and O

Results Improve for Zeus-2 and SB-5 but Then Deteriorate

RESULTS FOR IEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}			
		VI.8	VI.6	VI.4	VI.2
IEU-MF-03	1.0000±0.0017	0.9987±0.0003	0.9989±0.0003	0.9995±0.0003	1.0001±0.0003
BIG TEN	0.9948±0.0013	1.0071±0.0003	1.0071±0.0003	1.0088±0.0002	1.0043±0.0002
IEU-MF-04	1.0000±0.0030	1.0038±0.0003	1.0038±0.0003	1.0049±0.0003	1.0044±0.0003
Zebra-8H	1.0300±0.0025	1.0405±0.0002	1.0407±0.0002	1.0420±0.0003	1.0304±0.0002
IEU-CT-02	1.0017±0.0044	1.0007±0.0003	1.0003±0.0003	1.0012±0.0003	1.0010±0.0003
STACY-36	0.9988±0.0013	0.9988±0.0003	0.9985±0.0003	0.9964±0.0003	0.9964±0.0003

Introduction of Probability-Table Treatment for Unresolved Resonance Region Substantially Increases Reactivity for BIG TEN and Especially Zebra-8H

Reduction in 1/v Capture in H, Introduced in ENDF/B-VI.5, Is Primarily Responsible for Improvement in k_{eff} for STACY-36

RESULTS FOR LEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}			
		VI.8	VI.6	VI.4	VI.2
B&W XI-2	1.0007±0.0012	0.9968±0.0003	0.9968±0.0003	0.9987±0.0003	0.9965±0.0003
LEU-ST-02	1.0024±0.0037	0.99570.0003	0.9955±0.0003	0.9932±0.0003	0.9916±0.0003

Deterioration in k_{eff} for B&W XI-2 is Due Primarily to Changes to the ^{235}U Cross Sections Introduced in ENDF/B-VI.5

Reduction in 1/v Capture in H Is Primarily Responsible for Improvement in k_{eff} for LEU-ST-02

RESULTS FOR PU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}			
		VI.8	VI.6	VI.4	VI.2
Jezebel	1.0000±0.0020	0.9975±0.0003	0.9975±0.0003	0.9974±0.0003	0.9974±0.0003
Jezebel-240	1.0000±0.0020	0.9979±0.0003	0.9979±0.0003	0.9989±0.0003	0.9985±0.0003
Pu Buttons	1.0000±0.0030	0.9962±0.0003	0.9963±0.0003	0.9965±0.0003	0.9969±0.0003
Flattop-Pu	1.0000±0.0030	1.0019±0.0003	1.0019±0.0004	1.0031±0.0003	1.0032±0.0003
THOR	1.0000±0.0006	1.0062±0.0003	1.0062±0.0003	1.0058±0.0003	1.0062±0.0003
Pu-MF-11	1.0000±0.0010	0.9970±0.0003	0.9969±0.0003	0.9974±0.0003	0.9980±0.0004
HISS/HPG	1.0000±0.0110	1.0105±0.0003	1.0105±0.0002	1.0103±0.0002	1.0105±0.0002
PNL-33	1.0024±0.0021	1.0029±0.0003	1.0036±0.0003	1.0032±0.0003	1.0015±0.0003
PNL-2	1.0000±0.0065	1.0033±0.0005	1.0036±0.0005	1.0010±0.0005	1.0006±0.0005

Only Minor Reactivity Changes Occur for Any of These Cases

SUMMARY OF ENDF/B-VI RESULTS FOR MCNP CRITICALITY VALIDATION SUITE

Range	VI.8	VI.6	VI.4	VI.2
$\|\Delta k\| \leq \sigma$	13	12	10	13
$\sigma < \|\Delta k\| \leq 2\sigma$	9	10	11	12
$\|\Delta k\| > 2\sigma$	9	9	10	6

Overall, ENDF/B-VI.2 Produces Best Results

Results from Subsequent Releases Initially Deteriorate but Subsequently Improve

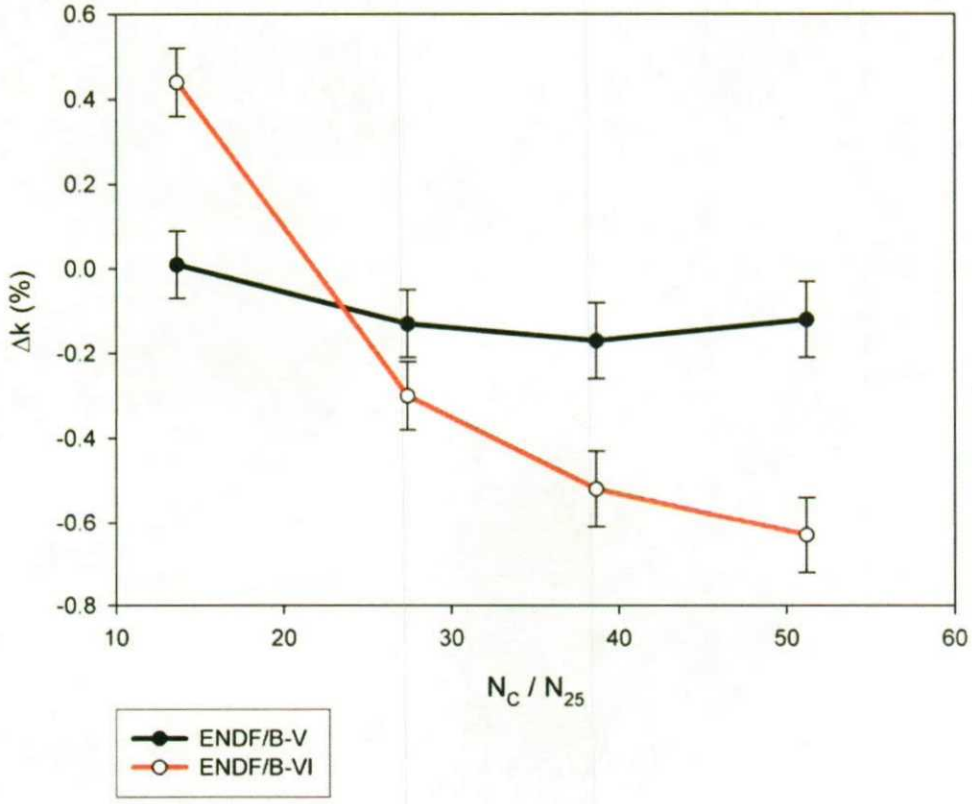
COMPARISON OF ENDF/B-V AND ENDF/B-VI RESULTS FOR MCNP CRITICALITY VALIDATION SUITE

Range	ENDF/B-VI.8	ENDF/B-V
$\|\Delta k\| \leq \sigma$	13	11
$\sigma < \|\Delta k\| \leq 2\sigma$	9	13
$\|\Delta k\| > 2\sigma$	9	7

ENDF/B-VI Produces 2 More Results within 1 Standard Deviation of the Benchmark Value but also 2 More Results That Differ from It by More Than 2 Standard Deviations

ENDF/B-VI Shows Marked Improvement for Thermal Plutonium Systems but Substantial Deterioration for Thermal ^{233}U and LEU Systems and for Intermediate HEU Systems

REACTIVITY BIASES FOR ZEUS CRITICAL EXPERIMENTS



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CONCLUSIONS

Overall, the Final Release of ENDF/B-VI Shows Marginal Improvement Relative to ENDF/B-V

Improvements Still Are Needed to the Cross Sections for a Number of Nuclides, Including ^{232}Th, ^{233}U, ^{235}U, ^{238}U, and ^{239}Pu

Better Agreement for Some of the Cases in the MCNP Criticality Validation Suite Could Be Obtained by Reverting to Cross Sections from Earlier Interim Releases for Certain Nuclides over Certain Energy Ranges, Such As

- ENDF/B-VI.6 Cross Sections for ^{16}O Would Improve k_{eff} for SB-2½, SB-5, and Godiver

- ENDF/B-VI.4 Cross Sections for ^{235}U in the Intermediate Energy Would Improve k_{eff} for UH_3 and Zeus-2