LA-UR-04-0876

Approved for public release; distribution is unlimited.

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

Author(s): Russell D. Mosteller

Submitted to: PHYSOR 2004: The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments
Chicago, IL
April 25 - 29, 2004

Los Alamos
NATIONAL LABORATORY

LA-UR-04-0876

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

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

The final release of version VI of the Evaluated Nuclear Data File (ENDF/B-VI) 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 the 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 ENDF/B-V and to earlier interim releases of ENDF/B-VI, the final release for ENDF/B-VI produces better agreement with benchmark values of k_{eff} for some cases but worse agreement for others. In addition, poor agreement with the benchmark values for the most extreme 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. In addition, agreement for some of the cases could be improved by retaining cross sections from earlier interim releases of ENDF/B-VI for certain nuclides over certain energy ranges.

PHYSOR 2004 - The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developements
Chicago, Illinois, April 25-29, 2004, on CD-ROM, American Nuclear Society, Lagrange Park, IL. (2004)

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

Russell D. Mosteller[1*]
[1] *Los Alamos National Laboratory, P. O. Box 1663, Los Alamos, NM 87545 USA*

The final release of version VI of the Evaluated Nuclear Data File (ENDF/B-VI) was distributed in October 2001. This study provides an assessment of the 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 ENDF/B-V, the final release for ENDF/B-VI produces better agreement with benchmark values of k_{eff} for some cases but worse agreement for others. In addition, poor agreement with the benchmark values for the most extreme cases remains essentially unaffected. Improvements still are needed in the cross sections for a number of nuclides, including ^{232}Th, ^{233}U, ^{235}U, ^{238}U, and ^{239}Pu.

KEYWORDS: ENDF/B-VI, MCNP, Criticality, Validation, Benchmarks

1 Introduction

The final release of version VI of the Evaluated Nuclear Data File [1], release 8 (ENDF/B-VI.8), was distributed in October 2001. That release came approximately two decades after the final release of its predecessor, ENDF/B-V [2]. 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 [3] and the benchmarks in the MCNP criticality validation suite.

1.1 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. The original suite [4] contained 26 benchmarks, but it subsequently has been expanded to 31. Five new cases have been added, and three others have been replaced. In two of the latter cases, benchmarks based on actual critical experiments replaced ones that were not (a subcritical extrapolation and a k_∞ measurement). The specifications for all 31 benchmarks are taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* [5].

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

* Corresponding author, Tel. 505-665-4879, FAX 505-665-3046, E-mail: mosteller@lanl.gov

The cases in the suite were selected to encompass a variety of fissile materials in configurations that produce fast, intermediate, and thermal spectra. The selected benchmarks include six cases with ^{233}U, 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. The suite includes cases with fast, intermediate, and thermal spectra for each fuel type except LEU, which of course can achieve criticality only with a thermal spectrum. The distribution of cases by fuel material, geometry, and spectrum is shown in Table 1, and a brief summary of each case is provided in Table 2.

1.2 ENDF/B-VI Nuclear Data Libraries

Based on different interim releases of ENDF/B-VI, four separate nuclear data libraries were generated for MCNP: ENDF60 [6], URES [7], ENDF66 [8], and ACTI [9]. The distinctions between those libraries are summarized in Table 3. Although earlier interim releases of ENDF/B-VI included delayed-neutron spectra and sufficient information for stratified sampling within the unresolved resonance region, URES was the first of these libraries to contain probability tables for the unresolved resonance region, and ENDF66 was the first to contain delayed-neutron spectra for fissioning nuclides. ACTI contains no actinides and was developed primarily for prompt γ-ray spectroscopy.

Because the ENDF/B-VI releases are cumulative, the smaller libraries can be combined with the larger ones to produce sets of nuclear data that correspond quite closely to specific releases. In particular, when the nuclides in URES supersede the corresponding ones in ENDF60, the resulting combined library corresponds very closely to ENDF/B-VI.4. Similarly, when the ACTI nuclides supersede their counterparts in ENDF66, the resulting combined library corresponds very closely to ENDF/B-VI.8, the final version of ENDF/B-VI. In addition to ENDF66 and ACTI, the SAB2002 library [10] of thermal scattering laws, $S(\alpha,\beta)$, was issued in 2002. Calculations reported herein that employ ENDF66 and/or ACTI also use SAB2002, while calculations with URES and/or ENDF60 use the earlier TMCCS library of thermal scattering laws.

2 Calculated Results

MCNP5 calculations were performed for each case in the MCNP criticality validation suite, using nuclear data corresponding to ENDF/B-VI.2, ENDF/B-VI.4, ENDF/B-VI.6, or ENDF/B-VI.8. With the exception of two of the benchmarks, each calculation employed a total of 550 generations with 10,000 neutrons per generation. The results from the first 50 generations were excluded from the statistics, and therefore the results for each of those cases are based on 5,000,000 active neutron histories. The two exceptions are SB-5 and Zebra-8H. Those two benchmarkss require substantially more computer time per history than the others, and so 350 generations rather than 550 generations were used for them. Even so, the standard deviations for k_{eff} from those cases are comparable to those for other benchmarks in the suite.

Results from those calculations are presented in Table 4 for the ^{233}U, HEU, and IEU benchmarks and in Table 5 for the LEU and plutonium benchmarks. Values for k_{eff} that differ from the benchmark value by more than two standard deviations are shown in red, while values that differ by more than one standard deviation but less than two are shown in blue.

Table 1 Distribution of cases in the MCNP criticality validation suite

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)†	SB-2½	ORNL-11
HEU	Godiva Tinkertoy-2 (c-11)	Flattop-25	Godiver	Zeus (2) UH_3 (6)	SB-5	ORNL-10
IEU	IEU-MF-03	BIG TEN	IEU-MF-04	Zebra-8H‡	IEU-CT-02 (3)	STACY-36
LEU					B&W 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

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

† Extrapolated to critical

‡ k_∞ measurement

Table 2 Summary of cases in the MCNP criticality validation suite

Case	Description
Jezebel-233	Bare sphere of ^{233}U
Flattop-23	Sphere of ^{233}U reflected by normal uranium
U233-MF-05 (2)	Sphere of ^{233}U reflected by beryllium
Falstaff (1)	Sphere of ^{233}U uranyl fluoride solution
SB-2½	Lattice of ^{233}U fuel pins in water
ORNL-11	Sphere of ^{233}U uranyl nitrate solution
Godiva	Bare sphere of HEU
Tinkertoy-2 (c-11)	3 x 3 x 3 array of HEU cylinders reflected by paraffin
Flattop-25	Sphere of HEU reflected by normal uranium
Godiver	Sphere of HEU reflected by water
Zeus (2)	Cylinder of HEU plates moderated by graphite and reflected by copper
UH_3 (6)	Stacked cylinders of HEU UH_3 reflected by depleted uranium
SB-5	Lattice of HEU pins in water surrounded by a blanket of ThO_2 pins
ORNL-10	Sphere of HEU uranyl nitrate solution
IEU-MF-03	Bare sphere of IEU (36 wt.%)
BIG TEN	Cylinder of IEU (10 wt.%) reflected by normal uranium
IEU-MF-04	Sphere of IEU (36 wt.%) reflected by graphite
Zebra-8H	Plate of IEU (37.5 wt.%) reflected by normal uranium and steel
IEU-CT-02 (3)	Lattice of IEU (17 wt.%) fuel rods in water
Stacy (36)	Cylinder of IEU (9.97 wt.%) uranyl nitrate solution
B&W XI (2)	Lattice of LEU (2.46 wt.%) UO_2 fuel pins in borated water
LEU-ST-02 (2)	Sphere of LEU (4.9 wt.%) uranyl fluoride solution
Jezebel	Bare sphere of plutonium
Jezebel-240	Bare sphere of plutonium (20.1 at.% ^{240}Pu)
Pu Buttons (3)	3 x 3 x 3 array of small cylinders of plutonium
Flattop-Pu	Plutonium sphere reflected by normal uranium
THOR	Plutonium sphere reflected by thorium
Pu-MF-11	Plutonium sphere reflected by water
HISS/HPG	Infinite, homogeneous mixture of plutonium, hydrogen, and graphite
PNL-33	Lattice of mixed-oxide fuel pins in borated water
PNL-2	Sphere of plutonium nitrate solution

2.1 ENDF/B-VI.2

The ENDF/B-VI.2 results constitute the baseline for this study. Relative to ENDF/B-V, ENDF/B-VI.2 generally produces lower values for k_{eff} , sometimes dramatically so [11]. Notable exceptions to that generalization are the three Flattop benchmarks, Jezebel, and Jezebel-240, for which the change in reactivity is small or insignificant. One obvious deficiency in both ENDF/B-V

Table 3 Characteristics of MCNP nuclear data libraries

Library	Issued	Source	Total Nuclides	Nuclides with Probability Tables	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

and ENDF/B-VI.2 is that they produce large reactivity swings between the bare metal spheres (Jezebel-233, Godiva, and Jezebel) and their Flattop counterparts.

2.2 ENDF/B-VI.4

Relative to ENDF/B-VI.2, ENDF/B-VI.4 produces large decreases in reactivity for the HEU and IEU cases with intermediate spectra and smaller changes for BIG TEN, Godiver, and the thermal uranium lattices. URES was the first MCNP library to incorporate an improved treatment for the unresolved resonance range, based on stratified sampling techniques. In fact, the reactivity changes for BIG TEN and Zebra-8H are due almost entirely to that enhancement. However, its net impact on reactivity is essentially limited to systems with substantial concentrations of nuclides with effective fission thresholds, such as ^{238}U or ^{240}Pu [12]. The reactivity changes for the other cases are produced primarily by changes to ^{235}U data in the epithermal energy range.

The reactivity changes that ENDF/B-VI.4 produces overall are mixed. Agreement with the benchmark value improves for one of the HEU case with an intermediate spectrum, Zeus (2), and for the thermal LEU lattice and solution. However, it deteriorates for the water-reflected HEU sphere and for the thermal ^{233}U and HEU lattices.

2.3 ENDF/B-VI.6

ENDF66 was the first of these libraries to include delayed-neutron spectra. However, the impact of that enhancement is fairly limited [13]. It produces relatively small reactivity changes for Falstaff (1), BIG TEN, and Zebra-8H, and it also produces small reactivity increases for UH_3 (6) and Zeus (2). However, it changes the reactivity by ± 0.001 Δk or less for the other cases in this study.

After the effects of delayed-neutron spectra are accounted for, the most notable reactivity changes from ENDF/B-VI.4 to ENDF/B-VI.6 involve the HEU cases with intermediate spectra, the thermal solutions, and some of the thermal lattices. The decreases in reactivity for UH_3 (6) and Zeus (2) result from changes to the cross sections for ^{235}U in the intermediate-energy range that were introduced in ENDF/B-VI.5. These reactivity changes would be even larger in the absence of delayed-neutron spectra, because those spectra increase reactivity for each of these two cases by approximately 0.001 Δk. k_{eff} for these two cases already was significantly lower than the benchmark value, and these changes to the ^{235}U cross sections exacerbate that difference.

Table 4 MCNP5 Results for ^{233}U, HEU, and IEU Benchmarks

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VI.8 (ACTI+ENDF66)	ENDF/B-VI.6 (ENDF66)	ENDF/B-VI.4 (URES+ENDF60)	ENDF/B-VI.2 (ENDF60)
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 (2)	1.0000 ± 0.0030	0.9976 ± 0.0003	0.9963 ± 0.0003	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
Godiva	1.0000 ± 0.0010	0.9962 ± 0.0003	0.9962 ± 0.0003	0.9967 ± 0.0003	0.9965 ± 0.0003
Tinkertoy-2 (c-11)	1.0000 ± 0.0038	0.9972 ± 0.0004	0.9972 ± 0.0004	0.9981 ± 0.0003	0.9987 ± 0.0003
Flattop-25	1.0000 ± 0.0030	1.0024 ± 0.0003	1.0024 ± 0.0003	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 (6)	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
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 (3)	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

*3,000,000 active histories

Table 5 MCNP5 Results for LEU and Plutonium Benchmarks

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VI.8 (ACTI+ENDF66)	ENDF/B-VI.6 (ENDF66)	ENDF/B-VI.4 (URES+ENDF60)	ENDF/B-VI.2 (ENDF60)
B&W XI (2)	1.0007 ± 0.0012	0.9968 ± 0.0003	0.9968 ± 0.0003	0.9987 ± 0.0003	0.9968 ± 0.0003
LEU-ST-002 (2)	1.0024 ± 0.0037	0.9957 ± 0.0003	0.9955 ± 0.0003	0.9932 ± 0.0003	0.9916 ± 0.0003
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 ± 0.0003	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

The reactivity increases for the solution benchmarks occur primarily because of a change to the radiative capture for hydrogen that also was introduced in ENDF/B-VI.5. Specifically, the 1/v portion of that cross section was reduced slightly and returned to its ENDF/B-V value. Although that change only amounted to 0.2%, it significantly reduces the thermal capture in aqueous solutions. For example, nearly 50% of all of the captures in ORNL-10 and ORNL-11 occur in hydrogen, and almost all of them occur at thermal energies. The same reduction is primarily responsible for the reactivity increases for the thermal ^{233}U and HEU lattices. However, the harder spectra for the other thermal lattices diminish the impact of that change.

2.4 ENDF/B-VI.8

The only difference between the ENDF/B-VI.6 and ENDF/B-VI.8 calculations is the use of the ACTI library. Except for tungsten, the ACTI library contains only nuclides with atomic numbers below 30. Consequently, the ENDF/B-VI.8 and ENDF/B-VI.6 calculations for several of these cases are identical.

The most noticeable reactivity changes for ENDF/B-VI.8 are the increase for the beryllium-reflected ^{233}U sphere and the decrease for the thermal lattice of HEU fuel pins. ENDF/B-VI.8 includes a revision to the radiative capture cross section for ^{9}Be that produces the small increase in reactivity for U233-MF-05 (2). Another revision in ENDF/B-VI.8 involves fairly substantial changes to the nuclear data for ^{16}O. These changes produce the reactivity loss for SB-5, and subsequent sensitivity studies demonstrated that they also reduce reactivity for SB-2½ and Godiver.

2.5 Summary of ENDF/B-VI REsults

The MCNP criticality validation suite should not be used as an absolute indicator of the accuracy or reliability of a nuclear data library. As the case names indicate, many of them are taken from sequences of similar benchmarks, and the sequence as a whole may display sensitivities that a single case cannot capture. Nonetheless, the suite can provide a general indication of the overall performance of a given library, and it can alert the user to unexpected or unintended consequences resulting from changes to nuclear data. In addition, it can help to identify areas where improvements are needed.

The agreement between the calculated and benchmark values for k_{eff} for the cases in the suite is summarized in Table 6. The Table shows no net improvement from ENDF/B-VI.2 to ENDF/B-VI.8. In fact, it indicates the contrary. ENDF/B-VI.2 and ENDF/B-VI.8 have the same number of cases for which k_{eff} is within one standard deviation of the benchmark value, but ENDF/B-VI.2 has three fewer cases where the difference exceeds two standard deviations.

Relative to ENDF/B-VI.2, ENDF/B-VI.8 produces better agreement with the benchmark values of k_{eff} for thermal solutions. However, the agreement has deteriorated slightly for the water-reflected metal spheres and the thermal lattices of ^{233}U and HEU fuel pins, and it has deteriorated significantly for the HEU cases with intermediate spectra. The reduction in reactivity for those cases results from the introduction of the ENDF/B-VI.5 changes to the ^{235}U cross sections in the intermediate-energy range, and those changes have been retained in ENDF/B-VI.8.

Other changes are due more to enhanced capabilities in the MCNP data libraries than to changes in the nuclear data *per se*. The inclusion of delayed-neutron spectra generates small changes for some cases, and the incorporation of probability-tables for the unresolved resonance range produces substantive changes for BIG TEN and some of the cases with intermediate spectra.

The progressive changes in the ENDF/B-VI releases do not produce much improvement for the most extreme cases. For all four releases, the differences between the calculated and benchmark

Table 6 Summary of Results for MCNP Criticality Validation Suite

Range	ENDF/B-VI.8 (ACTI+ENDF66)	ENDF/B-VI.6 (ENDF66)	ENDF/B-VI.4 (URES+ENDF60)	ENDF/B-VI.2 (ENDF60)
$\lvert\Delta k\rvert \leq \sigma$	13	12	10	13
$\sigma < \lvert\Delta k\rvert \leq 2\sigma$	9	10	11	12
$\lvert\Delta k\rvert > 2\sigma$	9	9	10	6

values for k_{eff} exceeds two standard deviations for four of the cases in the suite: Jezebel-233, Godiva, BIG TEN, and THOR. The only one of these cases for which the calculated value of k_{eff} changes appreciably is BIG TEN, and ENDF/B-VI.2 produces the best result for it. There are four additional cases for which the difference exceeds two standard deviations for all releases except ENDF/B-VI.2: Godiver, Zeus (2), Zebra-8H, and Pu-MF-11. The changes to the calculated values of k_{eff} for these cases from ENDF/B-VI.4 through the ENDF/B-VI.8 are quite small, except for Zeus (2). For that case, once again, the earliest of those results (ENDF/B-VI.4) produces the best agreement with the benchmark value.

One of the problems noted with ENDF/B-VI.2 in section 2.1 is the reactivity swing from the three bare metal spheres to their Flattop counterparts. That reactivity discrepancy exceeds 0.005 Δk for all three cases, and its magnitude remains essentially undiminished for all of the subsequent releases, including the final one.

Collectively, the results presented in Tables 4 and 5 suggest that the cross sections for a number of nuclides still need improvement. Adjustments to the cross sections for ^{238}U conceivably could produce better values for k_{eff} for BIG TEN, Zebra-8H, and B&W XI (2). Improved cross sections also are needed for ^{233}U, ^{235}U, ^{239}Pu, and possibly ^{238}U to improve the results for the bare metal spheres and produce better consistency with their Flattop counterparts. Similarly, improvements to the cross sections for ^{232}Th could produce a better value for k_{eff} for THOR and possibly for SB-5 as well, because it has thorium rods in its blanket region. Better agreement with the benchmark values might also result from returning to cross sections from earlier interim releases for certain nuclides over certain energy ranges. For example, reversion to the ENDF/B-VI.6 cross sections for ^{16}O would improve the results for SB-2½, SB-5, and Godiver, and returning to the ENDF/B-VI.4 cross sections for ^{235}U in the intermediate energy range would improve k_{eff} for Zeus (2) and UH_3 (6).

3 Comparison of ENDF/B-VI and ENDF/B-V REsults

In the end, the fundamental question is whether ENDF/B-VI produces more accurate and reliable results than ENDF/B-V does. The answer, as Table 7 indicates, is that it sometimes produces better results, it sometimes produces worse results, and it sometimes produces essentially the same results. Overall, ENDF/B-VI produces results that are within one standard deviation of the benchmark value of k_{eff} for 13 of the cases, compared to 11 of the cases for ENDF/B-V. However, It also has more cases where that difference exceeds two standard deviations, nine versus seven.

ENDF/B-VI produces improved results for two of the three Flattop cases, for the bare IEU sphere and the IEU sphere reflected by beryllium, and for both of the thermal plutonium cases. However,

Table 7 Comparison of MCNP5 Results with ENDF/B-VI and ENDF/B-V

Case	Benchmark k_{eff}	Calculated k_{eff}	
		ENDF/B-VI	ENDF/B-V
Jezebel-233	1.0000 ± 0.0010	0.9931 ± 0.0002	0.9930 ± 0.0003
Flattop-23	1.0000 ± 0.0014	1.0003 ± 0.0003	1.0016 ± 0.0003
U233-MF-05 (2)	1.0000 ± 0.0030	0.9976 ± 0.0003	0.9968 ± 0.0003
Falstaff (1)	1.0000 ± 0.0083	0.9894 ± 0.0005	0.9864 ± 0.0005
SB-2½	1.0000 ± 0.0024	0.9967 ± 0.0005	1.0007 ± 0.0005
ORNL-11	1.0006 ± 0.0029	0.9968 ± 0.0002	0.9987 ± 0.0002
Godiva	1.0000 ± 0.0010	0.9962 ± 0.0003	0.9979 ± 0.0003
Tinkertoy-2 (c-11)	1.0000 ± 0.0038	0.9972 ± 0.0004	0.9983 ± 0.0003
Flattop-25	1.0000 ± 0.0030	1.0024 ± 0.0003	1.0036 ± 0.0003
Godiver	0.9985 ± 0.0011	0.9948 ± 0.0003	0.9968 ± 0.0003
UH_3 (6)	1.0000 ± 0.0047	0.9914 ± 0.0003	0.9943 ± 0.0003
Zeus (2)	0.9997 ± 0.0008	0.9942 ± 0.0003	0.9992 ± 0.0004
SB-5*	1.0015 ± 0.0028	0.9963 ± 0.0005	0.9963 ± 0.0006
ORNL-10	1.0015 ± 0.0026	0.9992 ± 0.0002	1.0000 ± 0.0002
IEU-MF-03	1.0000 ± 0.0017	0.9987 ± 0.0003	1.0053 ± 0.0003
BIG TEN	0.9948 ± 0.0013	1.0071 ± 0.0003	1.0029 ± 0.0002
IEU-MF-04	1.0000 ± 0.0030	1.0038 ± 0.0003	1.0088 ± 0.0003
Zebra-8H*	1.0300 ± 0.0025	1.0405 ± 0.0002	1.0202 ± 0.0002
IEU-CT-02 (3)	1.0017 ± 0.0044	1.0007 ± 0.0003	1.0023 ± 0.0003
STACY-36	0.9988 ± 0.0013	0.9988 ± 0.0003	1.0002 ± 0.0003
B&W XI (2)	1.0007 ± 0.0012	0.9968 ± 0.0003	0.9984 ± 0.0003
LEU-ST-02 (2)	1.0024 ± 0.0037	0.9957 ± 0.0003	0.9964 ± 0.0003
Jezebel	1.0000 ± 0.0020	0.9975 ± 0.0003	0.9977 ± 0.0003
Jezebel-240	1.0000 ± 0.0020	0.9979 ± 0.0003	0.9987 ± 0.0003
Pu Buttons	1.0000 ± 0.0030	0.9962 ± 0.0003	0.9959 ± 0.0003
Flattop-Pu	1.0000 ± 0.0030	1.0019 ± 0.0003	1.0026 ± 0.0003
THOR	1.0000 ± 0.0006	1.0062 ± 0.0003	1.0049 ± 0.0003
Pu-MF-011	1.0000 ± 0.0010	0.9970 ± 0.0003	1.0007 ± 0.0004
HISS/HPG	1.0000 ± 0.0110	1.0105 ± 0.0003	1.0007 ± 0.0002
PNL-33	1.0024 ± 0.0021	1.0029 ± 0.0003	1.0077 ± 0.0003
PNL-2	1.0000 ± 0.0065	1.0033 ± 0.0005	1.0081 ± 0.0004

* 3,000,000 active neutron histories

it produces worse results for the thermal ^{233}U cases and the thermal lattice of LEU fuel pins. It also produces worse results for the bare HEU sphere, both of the water-reflected metal spheres, both HEU cases with intermediate spectra, and the IEU cylinder reflected by normal uranium. Although the inclusion of delayed-neutron spectra and probability tables for the intermediate energy range would have affected the ENDF/B-V results for some of these cases, the impact would not have been large enough to change the overall pattern.

4 Summary and Conclusions

The final release of ENDF/B-VI, ENDF/B-VI.8, shows improvements relative to ENDF/B-V and the early interim releases of ENDF/B-VI for some cases in the MCNP criticality validation suite, but it produces worse results for others. Specifically, it has more cases with values for k_{eff} within one standard deviation of the benchmark value than ENDF/B-V does, but it also has more cases for which that difference exceeds two standard deviations. Agreement for some of the cases could be improved by retaining cross sections from earlier interim releases of ENDF/B-VI for certain nuclides over certain energy ranges. On the whole, however, the results from this study strongly indicate that improvements still are needed in the cross sections for a number of nuclides, including ^{232}Th, ^{233}U, ^{235}U, ^{238}U, and ^{239}Pu.

Acknowledgements

This research was performed at Los Alamos National Laboratory under the auspices of contract W-7405-ENG-36 with the U. S. Department of Energy.

References

1) P. F. Rose, Ed., "ENDF-201, ENDF/B-VI Summary Documentation," BNL-NCS-17541, 4th Edition, Brookhaven National Laboratory (October 1991).
2) R. Kinsey, Ed., "ENDF-201, ENDF/B Summary Documentation," BNL-NCS-17541, 3rd Edition, Brookhaven National Laboratory (1979).
3) 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 Laboratory (April 2003).
4) Russell D. Mosteller, "Validation Suites for MCNP™," Proc. 12th Biennial Topl. Mtg. Radiation Protection and Shielding Div., Santa Fe, New Mexico, April 14-18, 2002 (2002).
5) *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, NEA/NSC/DOC(95)03, OECD Nuclear Energy Agency (Rev., 2003).
6) J. S. Hendricks, S. C. Frankle, and J. D. Court, "ENDF/B-VI Data for MCNP," LA-12891, Los Alamos National Laboratory (December 1994).
7) R. C. Little and R. E. MacFarlane, "ENDF/B-VI Neutron Library for MCNP with Probability Tables," LA-UR-98-5718, Los Alamos National Laboratory (December 1998).
8) Joann M. Campbell, Stephanie C. Frankle, and Robert 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 14-18, 2002 (2002).
9) Stephanie C. Frankle, Robert C. Reedy, and Phillip G. Young, "ACTI: An MCNP Data Library for Prompt Gamma-Ray Spectroscopy," Proc. 12th Biennial Topl. Mtg. Radiation Protection and Shielding Div., Santa Fe, New Mexico, April 14-18, 2002 (2002).

10) R. C. Little and R. E. MacFarlane, "SAB2002—An S(α,β) Library for MCNP," X-5-03-21(U), Los Alamos National Laboratory (February 3, 2003).
11) Russell D. Mosteller, Stephanie C. Frankle, and Phillip G. Young, "Data Testing of ENDF/B-VI with MCNP: Critical Experiments, Thermal Reactor Lattices, and Time-of-Flight Measurements," Adv. Nucl. Sci. Tech., **24**, pp. 131-195 (1997).
12) Russell D. Mosteller and Robert C. Little, "Impact of MCNP Unresolved Resonance Probability-Table Treatment on Uranium and Plutonium Lattices," Proc. Sixth Int. Conf. Nuclear Criticality Safety (ICNC 99), Vol. 2, pp. 522-531, Versailles, France, September 20-24, 1999 (1999).
13) Russell D. Mosteller and Christopher J. Werner, "Reactivity Impact of Delayed-Neutron Spectra on MCNP Calculations," Trans. Am. Nucl. Soc., **82**, 235 (June 2000).