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Comparison of Criticality Results for the ENDF60 and ENDF66 Libraries

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I. Introduction

ENDF66[1] is a continuous-energy neutron data library, formatted for use with MCNP version 4C or later.[2] The library contains data for 173 nuclides based on ENDF/B-VI (Release 6) evaluations of the Cross Section Evaluation Working Group (CSEWG)[3] and was processed with the NJOY99 code.[4]

This library succeeds the ENDF60[5] library (based on ENDF/B-VI, Release 2), the URES library[6] (based on ENDF/B-VI, Release 4, and including unresolved-resonance probability tables), and the ENDF6DN library[7] (ENDF60 data with delayed-neutron spectral data appended). Since the last comprehensive MCNP library, ENDF60, was released by LANL in June 1993, several important new evaluations have been performed and the MCNP data library format has been expanded allowing for new data, including delayed-neutron spectra, unresolved-resonance probability tables, detailed charged-particle production, and tabular angular distributions. Relative to the ENDF60 library, the new ENDF66 library has added 58 new nuclides and data for 40 nuclides are based on new evaluations. In particular, updated evaluations for uranium, plutonium, tungsten, and iron isotopes have been performed. Additionally, some changes from ENDF60 have been made in NJOY processing, including the use of smaller resonance reconstruction tolerances and decreased thinning of energy points.

Data for all nuclides were processed at 293.6K. Additionally, nuclides having unresolved-resonance data were processed at 3000K and 35 nuclides include data processed at 77K. MCNP version 4C or later is required for performing simulations with the ENDF66 libraries.

As part of the ongoing validation process for the ENDF66 library, the data library was used in a series of criticality benchmark calculations. Here we present k_{eff} results from a set of criticality benchmarks for the ENDF60 library, the ENDF66 libraries, and the ENDF66 libraries without unresolved-resonance data. The *phys:n* parameters in MCNP are used to control the use of both the unresolved-resonance and delayed-neutron spectral data. Both types of data are used, or turned on, by default in MCNP4C and later.

II. Criticality Benchmarks

A comprehensive suite of 86 criticality benchmarks has been run using room-temperature data from ENDF66.[8] Benchmark specifications were taken from the International Criticality Safety Benchmark Evaluation Project (ICSBEP)[9] and the Cross Section Evaluation Working Group (CSEWG) specifications.[10] From these compilations, a subset of benchmarks was chosen that tests a wide range of energy regions and a variety of important reflector materials, although the benchmark suite by no means covers all isotopes and energy regions of interest. In particular, suitable benchmarks for intermediate-energy critical assemblies, low-enrichment uranium metal assemblies, and assemblies using ^{232}Th are lacking. Categorized by fissile material, the benchmark assemblies fall into one of five main groups: ^{233}U, intermediate-enriched ^{235}U (IEU), highly enriched ^{235}U (HEU), ^{239}Pu, and mixed metal.

There are two sets of specifications for five of the critical assemblies. For Flattop-23, a sphere of ^{233}U reflected by normal uranium, the CSEWG specification (*flat23*) contains a small gap between the main fuel and the reflector, whereas the ICSBEP specification has no gap (*23umt6*). ICSBEP specifications for Godiva contain both the standard sphere of HEU (*umet1ss*) as well as nested spherical shells of HEU (*umet1ns*). There are two specifications for the one- and two-dimensional models for Bigten (*bigten1* and *bigten2*), and for the water-reflected sphere of HEU (*umet4a* and *umet4b*). The thorium-reflected sphere of ^{239}Pu, Thor, also has a one- and two-dimensional representation (*pumet8a* and *pumet8b*). Therefore, there are a total of 91 MCNP input files and corresponding benchmark results.

III. Benchmark k_{eff} Results

This report focuses only on the results of k_{eff} criticality calculations. The benchmarks were calculated using both the ENDF66 (with and without probability tables) and ENDF60 libraries. Benchmark results for ENDF60 data were previously reported in Ref.11. For this comparison, these benchmarks were performed again for ENDF60 on the SGI Origin 2000 platform using MCNP4C2. The ENDF66 results with no probability tables were also calculated on an SGI Origin 2000 platform using MCNP4C2. The ENDF66 results with probability tables were calculated on the LAMBDA cluster at LANL (cluster of Compaq DL360 with two Intel Pentium-3, 1 GHz processors running RedHat Linux) using MCNP5 (1.7). In all cases, substantial increases in the number of active cycles were included compared to results reported in Ref. 11. A recently completed study verifies that MCNP4C and MCNP5 give the same results for kcode calculations run on the same platform.[12]

Tables 1-13 show the results of the benchmark calculations. The results are quoted with 2σ uncertainties, representing a confidence level of 95% that the true k_{eff} for the calculations lies within the quoted range. The ENDF60 data have no unresolved-resonance data and no delayed-neutron spectral data. The benchmarks were run twice using ENDF66 data to better understand the impact of the unresolved-resonance probability tables: once using the probability tables (labeled "ENDF66 with PT" in Tables 1-13) and again without using unresolved-resonance probability tables (labeled "ENDF66 without PT"). Delayed-neutron spectral data were used for both ENDF66 runs.

The benchmark results are presented in 13 groups: bare metal assemblies, solution experiments, water-reflected metal assemblies, assemblies reflected by polyethylene, beryllium and beryllium oxide, graphite, aluminum, steel and nickel, tungsten, thorium, normal uranium, and HEU, and other experiments. For a more complete description of the benchmarks, refer to Ref. 8.

IV. Discussion of Benchmark Results

There is a trend for the ENDF66 data to calculate a slightly lower value for k_{eff} than for the ENDF60 data for the bare metal assemblies in Table 1 and the water-reflected, the poly-reflected, the beryllium and beryllium-oxide reflected, the graphite-reflected, the aluminum-reflected, and the steel and nickel-reflected assemblies in Tables 3-8. The addition of probability table data does not significantly impact these results.

It can be seen from Table 2 that k_{eff} of solution assemblies has tended to increase with use of the ENDF66 data for ^{233}U and ^{235}U systems. Several significant changes from ENDF60 results are seen particularly in the uranium solutions, bringing the calculated result closer to the quoted benchmark result. The results for the ^{239}Pu solutions are essentially unchanged from ENDF60 and tend to slightly overpredict k_{eff}.

In Table 9 the results for the tungsten-carbide-reflected assemblies show that both ENDF60 and ENDF66 calculate too high of a value. Additionally, the results for *umet3h-k*, show a correlation in amount of change in k_{eff} with the reflector thickness between the two libraries. The assembly with the thinnest reflector (*umet3h*) showed the largest decrease in k_{eff}, relative to ENDF60 and the assembly with the thickest reflector (*umet3k*) showed the largest increase. We can see that this trend is completely driven by the probability tables. The ENDF66 results calculated without probability-table processing show no significant change from the ENDF60 results.

The thorium-reflected assembly in Table 10 shows that ENDF66 calculates high as did ENDF60. The addition of probability table data does not significantly impact these results.

The trend of the normal U-reflected assemblies in Table 11 shows a modest decrease in k_{eff} for ENDF66. However, *bigten1* and *bigten2* show a significant increase in k_{eff}. We see here, as was noted by Mosteller and Little, that the use of probability tables has a significant impact on the results of these two benchmarks. However, ENDF66 results for *bigten* show a marked improvement relative to experiment over the results based on ENDF/B-VI Release 4 from Ref.13.

The results in Table 12 show that ENDF66 calculates low for HEU-reflected assemblies, as did ENDF60. The addition of probability table data does not significantly impact these results. The same conclusion can be drawn from the *ieumt* assemblies in Table 13, but there is a dramatic difference for the *mixmet8* assembly.

In Table 13 the benchmark *mixmet8* shows a significant increase for ENDF66 k_{eff}. We can see, though, that this change is because of the addition of the probability tables (in particular for ^{238}U). Unfortunately, the ENDF66 result with probability tables show the most discrepancy with the experimental value of 0.992. *mixmet8* is a graphite- and uranium-reflected assembly that has a substantial part of the neutron flux in the intermediate-energy range where probability table data would have the greatest impact. Reference 11 has an extensive discussion of the flux spectra in the various material regions. In comparison with the ENDF/B-V result of 0.9591±0.0009 discussed in reference 11, all of the ENDF/B-VI data show much improvement.

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Table 1: Criticality Benchmark Results for Bare Metal Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
23umt1	Jezebel-23	U-233	1.000±0.001	0.9931±0.0003	0.9934±0.0003	0.9928±0.0003
ieumt3		IEU (36 wt.%)	1.0000±0.0017	1.0001±0.0004	0.9992±0.0004	0.9997±0.0004
umet1ss	Godiva	HEU	1.000±0.001	0.9968±0.0003	0.9964±0.0003	0.9966±0.0003
umet1ns	Godiva	HEU	1.000±0.001	0.9966±0.0004	0.9968±0.0003	0.9962±0.0003
umet8		HEU	0.9989±0.0016	0.9927±0.0004	0.9922±0.0003	0.9927±0.0003
umet15		HEU	0.9996±0.0017	0.9917±0.0004	0.9914±0.0004	0.9913±0.0003
umet18		HEU	1.0000±0.0016	0.9962±0.0003	0.9960±0.0003	0.9960±0.0004
pumet1	Jezebel	Pu-239 (4.5% Pu-240)	1.000±0.002	0.9980±0.0003	0.9974±0.0003	0.9977±0.0003
pumet2	Jezebel	Pu-239 (20% Pu-240)	1.000±0.002	0.9988±0.0003	0.9976±0.0003	0.9983±0.0003
pumet22		Pu-239 (98)	1.0000±0.0021	0.9967±0.0003	0.9961±0.0003	0.9957±0.0003

Table 2: Criticality Benchmark Results for Solution Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
23usl1a	ORNL-5	U-233	1.0000±0.0031	0.9972±0.0002	0.9984±0.0002	0.9983±0.0002
23usl1b	ORNL-6	U-233	1.0005±0.0033	0.9973±0.0002	0.9983±0.0002	0.9983±0.0002
23usl1c	ORNL-7	U-233	1.0006±0.0033	0.9968±0.0002	0.9978±0.0002	0.9979±0.0002
23usl1d	ORNL-8	U-233	0.9998±0.0033	0.9967±0.0002	0.9977±0.0002	0.9977±0.0002
23usl1e	ORNL-9	U-233	0.9999±0.0033	0.9960±0.0002	0.9970±0.0002	0.9972±0.0002
23usl8	ORNL-11	U-233	1.0006±0.0029	0.9961±0.0002	0.9972±0.0002	0.9971±0.0002
usol13a	ORNL-1	HEU	1.0012±0.0026	0.9972±0.0002	0.9990±0.0002	0.9990±0.0002
usol13b	ORNL-2	HEU	1.0007±0.0036	0.9964±0.0002	0.9980±0.0002	0.9976±0.0002
usol13c	ORNL-3	HEU	1.0009±0.0036	0.9930±0.0003	0.9943±0.0003	0.9941±0.0003
usol13d	ORNL-4	HEU	1.0003±0.0036	0.9948±0.0003	0.9954±0.0003	0.9960±0.0003
usol32	ORNL-10	HEU	1.0015±0.0026	0.9970±0.0002	0.9985±0.0002	0.9987±0.0002
pnl1	PNL-1	Pu-239	1.0 (a)	1.0070±0.0004	1.0079±0.0004	1.0079±0.0004
pnl6	PNL-6	Pu-239	1.0 (a)	1.0016±0.0004	1.0020±0.0004	1.0019±0.0004
pusl11a	PNL-3	Pu-239	1.0000±0.0052	0.9947±0.0003	0.9954±0.0003	0.9956±0.0003
pusl11b	PNL-4	Pu-239	1.0000±0.0052	1.0001±0.0003	1.0001±0.0003	1.0007±0.0003
pusl11c	PNL-5	Pu-239	1.0000±0.0052	1.0051±0.0004	1.0054±0.0004	1.0059±0.0004
pusl11d		Pu-239	1.0000±0.0052	1.0091±0.0004	1.0098±0.0004	1.0105±0.0004

(a) Specific benchmark values were not given in the CSEWG specifications, and are assumed to be 1.0.

Table 3: Criticality Benchmark Results for Water-Reflected Metal Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
umet4a		HEU (97.675)	1.002	1.0009±0.0004	1.0003±0.0004	1.0002±0.0004
umet4b		HEU (97.675)	1.0003±0.0005	0.9968±0.0004	0.9958±0.0004	0.9966±0.0004
pumet11		Pu-239	1.0000±0.001	0.9982±0.0004	0.9972±0.0004	0.9978±0.0004

Table 4: Criticality Benchmark Results for Polyethylene-Reflected Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
umet11		HEU (~89.6)	1.000±0.001	0.9970±0.0004	0.9954±0.0004	0.9952±0.0004
umet20		HEU	1.0000±0.0030	0.9975±0.0004	0.9967±0.0004	0.9969±0.0004
pumet24		Pu-239	1.0000±0.0020	1.0001±0.0004	0.9995±0.0004	0.9996±0.0004

Table 5: Criticality Benchmark Results for Beryllium and Beryllium-Oxide-Reflected Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
Be-Reflected						
23umt5a	Planet	U-233	1.0000±0.0030	0.9950±0.0004	0.9947±0.0004	0.9945±0.0004
23umt5b	Planet	U-233	1.0000±0.0030	0.9969±0.0004	0.9969±0.0004	0.9974±0.0004
umet9a		HEU (~89.6)	0.9992±0.0015	0.9949±0.0004	0.9950±0.0004	0.9949±0.0004
pumet18	Planet	Pu-239 (94.79)	1.0000±0.0030	0.9997±0.0004	0.9995±0.0004	0.9997±0.0004
pumet19		Pu-239 (~90)	0.9992±0.0015	1.0018±0.0004	1.0012±0.0004	1.0013±0.0004
pumt21a		Pu-239	1.0000±0.0026	1.0047±0.0004	1.0040±0.0004	1.0047±0.0004
BeO-Reflected						
umet9b		HEU (~89.6)	0.9992±0.0015	0.9937±0.0004	0.9938±0.0004	0.9937±0.0004
pumt21b		Pu-239	1.0000±0.0026	0.9929±0.0004	0.9925±0.0004	0.9929±0.0004

Table 6: Criticality Benchmark Results for Graphite-Reflected Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
ieumt4		IEU (36 wt.%)	1.0000±0.0030	1.0046±0.0004	1.0037±0.0004	1.0040±0.0004
umet19		HEU	1.0000±0.0030	1.0035±0.0004	1.0033±0.0004	1.0033±0.0004
pumet23		Pu-239	1.0000±0.0020	0.9982±0.0004	0.9978±0.0004	0.9980±0.0004

Table 7: Criticality Benchmark Results for Aluminum-Reflected Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
ieumt6		IEU (36 wt.%)	1.0000±0.0023	0.9922±0.0004	0.9914±0.0004	0.9916±0.0004
umet12		HEU(~89.6)	0.9992±0.0018	0.9933±0.0004	0.9937±0.0004	0.9933±0.0003
umet22		HEU	1.0000±0.0021	0.9920±0.0004	0.9921±0.0004	0.9924±0.0004
pumet9	Comet	Pu-239 (94.8)	1.0000±0.0027	1.0010±0.0004	1.0013±0.0004	1.0016±0.0004

Table 8: Criticality Benchmark Results for Steel- and Nickel-Reflected Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
Fe-Reflected						
ieumt5		IEU (36 wt.%)	1.0000±0.0021	0.9999±0.0004	0.9988±0.0004	0.9990±0.0004
umet13		HEU (~89.6)	0.9990±0.0015	0.9942±0.0004	0.9939±0.0004	0.9941±0.0004
umet21		HEU	1.0000±0.0026	0.9948±0.0004	0.9947±0.0004	0.9944±0.0004
pumet25		Pu-239	1.0000±0.0020	0.9967±0.0004	0.9966±0.0003	0.9972±0.0004
pumet26		Pu-239	1.0000±0.0024	0.9972±0.0004	0.9968±0.0004	0.9971±0.0004
Ni-Reflected						
umet3l	Topsy	HEU (93.5)	1.0000±0.0030	1.0048±0.0004	1.0044±0.0004	1.0044±0.0004

Table 9: Criticality Benchmark Results for Tungsten-Reflected Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
23umt4a	Planet	U-233	1.0000±0.0007	1.0028±0.0004	1.0021±0.0004	1.0024±0.0004
23umt4b	Planet	U-233	1.0000±0.0008	1.0052±0.0004	1.0037±0.0004	1.0050±0.0004
umet3h	Topsy	HEU (93.5)	1.0000±0.0050	1.0063±0.0004	1.0047±0.0004	1.0058±0.0004
umet3i	Topsy	HEU (93.5)	1.0000±0.0050	1.0064±0.0004	1.0059±0.0004	1.0063±0.0004
umet3j	Topsy	HEU (93.5)	1.0000±0.0050	1.0074±0.0004	1.0091±0.0004	1.0074±0.0004
umet3k	Topsy	HEU (93.5)	1.0000±0.0050	1.0095±0.0004	1.0131±0.0004	1.0091±0.0004
pumet5	Planet	Pu-239 (94.79)	1.0000±0.0013	1.0098±0.0004	1.0078±0.0004	1.0087±0.0004

Table 10: Criticality Benchmark Results for Thorium-Reflected Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
pumet8a	Thor (1D)	Pu-239 (93.59)	1.0000±0.0030	1.0068±0.0004	1.0062±0.0004	1.0065±0.0004
pumet8b	Thor (2D)	Pu-239 (93.59)	1.000±0.0006	1.0060±0.0004	1.0056±0.0004	1.0061±0.0004

Table 11: Criticality Benchmark Results for Normal Uranium-Reflected Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
23umt3a	Planet	U-233	1.0000±0.0010	0.9968±0.0003	0.9959±0.0003	0.9965±0.0004
23umt3b	Planet	U-233	1.0000±0.0010	0.9992±0.0004	0.9978±0.0004	0.9984±0.0004
23umt6	Flattop-23	U-233	1.0000±0.0014	1.0009±0.0004	1.0005±0.0004	1.0003±0.0004
flat23	Flattop-23	U-233	1.000±0.001	1.0027±0.0004	1.0025±0.0004	1.0018±0.0004
ieumt2	Jemima	IEU	1.000±0.003	1.0041±0.0003	1.0035±0.0003	1.0027±0.0003
umet3a	Topsy	HEU (93.5)	1.0000±0.0050	0.9927±0.0004	0.9916±0.0004	0.9923±0.0004
umet3b	Topsy	HEU (93.5)	1.0000±0.0050	0.9929±0.0004	0.9915±0.0004	0.9923±0.0004
umet3c	Topsy	HEU (93.5)	1.0000±0.0050	0.9984±0.0004	0.9966±0.0004	0.9975±0.0004
umet3d	Topsy	HEU (93.5)	1.0000±0.0030	0.9965±0.0004	0.9952±0.0004	0.9960±0.0004
umet3e	Topsy	HEU (93.5)	1.0000±0.0030	1.0007±0.0004	1.0005±0.0004	1.0002±0.0004
umet3f	Topsy	HEU (93.5)	1.0000±0.0030	1.0012±0.0004	1.0010±0.0004	1.0003±0.0004
umet3g	Topsy	HEU (93.5)	1.0000±0.0030	1.0021±0.0004	1.0015±0.0004	1.0013±0.0004
umet14		HEU (~89.6)	0.9989±0.0017	0.9954±0.0004	0.9942±0.0004	0.9950±0.0004
umet28	Flattop-25	HEU	1.0000±0.0030	1.0027±0.0004	1.0019±0.0004	1.0016±0.0004
bigten1	Bigten	HEU	0.996±0.003	1.0067±0.0003	1.0092±0.0003	1.0046±0.0003
bigten2	Bigten	HEU	0.996±0.003	1.0046±0.0003	1.0072±0.0003	1.0023±0.0003
pumet6	Flattop	Pu-239 (93.80)	1.0000±0.0030	1.0040±0.0004	1.0028±0.0004	1.0028±0.0004
pumet10		Pu-239	1.0000±0.0018	1.0001±0.0004	0.9986±0.0004	0.9995±0.0004
pumet20		Pu-239 (~90)	0.9993±0.0017	0.9998±0.0004	0.9985±0.0004	0.9986±0.0004

Table 12: Criticality Benchmark Results for Highly Enriched Uranium-Reflected Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
23umt2a	Planet	U-233	1.0000±0.0010	0.9957±0.0003	0.9957±0.0003	0.9953±0.0003
23umt2b	Planet	U-233	1.0000±0.0011	0.9978±0.0003	0.9974±0.0003	0.9978±0.0003
mixmet1	Planet	Mixed Metal (Pu)	1.0000±0.0016	0.9972±0.0004	0.9966±0.0004	0.9967±0.0003
mixmet3		Mixed Metal (Pu)	0.9993±0.0016	0.9988±0.0004	0.9984±0.0004	0.9984±0.0004

Table 13: Criticality Benchmark Results for Other Assemblies

MCNP Filename	Assembly Name	Material	Benchmark k_{eff}	ENDF60	ENDF66 with PT	ENDF66 without PT
ieumt1a	Jemima 1	HEU & U(nat)	0.9989	0.9974±0.0004	0.9964±0.0004	0.9966±0.0004
ieumt1b	Jemima 2	HEU & U(nat)	0.9997	0.9969±0.0004	0.9971±0.0004	0.9968±0.0004
ieumt1c	Jemima 3	HEU & U(nat)	0.9993	0.9988±0.0004	0.9978±0.0004	0.9984±0.0004
ieumt1d	Jemima 4	HEU & U(nat)	1.0002	0.9998±0.0004	0.9986±0.0004	0.9989±0.0004
mixmet8	Zebra 8A/2	Pu w/graphite & U(nat) reflector	0.9920±0.0063	0.9922±0.0003	1.0044±0.0003	0.9930±0.0003