k_{eff}, Reaction Rates and Spectral Measurements in Critical Assemblies

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Abstract

Recently, a suite of 86 criticality benchmarks for MCNP was developed and the results of testing the ENDF/B-V and ENDF/B-VI data (through Release 2) were published (LA-13594 and LA-13627). In addition to the standard k_{eff} measurements, a number of these benchmarks also had other experimental measurements performed on the assemblies. In particular, the CSEWG specifications contain experimental data for neutron leakage and central-flux measurements, central-fission ratio measurements, and activation ratio measurements. This presentation will present the results for the k_{eff} measurements for the ENDF/B-V, ENDF/B-VI and ENDL92 data libraries using MCNP.

Critical Assemblies

- k_{eff}
  - 86 critical assemblies
- Neutron Central-flux and Leakage Spectra
  - Jezebel, Jezebel-23, Godiva, and Bigten
- Central Reaction Rates
  - Fission, (n,γ), (n,α), (n,p), (n,2n), (n,n'γ)

Validating Nuclear Data

- 3 databases for neutron transport calculations
  - ENDF/B-V (early-mid 1980's, .50c and .55c)
  - ENDF/B-VI Release 2 (early 1990's, .60c)
  - ENDL92 - LLNL (.42c)
- Continuous-energy data libraries
  - Best representation of the evaluations
- Monte Carlo code MCNP

ENDF Evaluations

- Most ENDF/B-VI.2 evaluations are new. Those that remained unchanged are: ^{27}Al, Ga, ^{182,183,184,186}W, ^{232}Th, ^{233,234}U, and ^{242}Pu
- The only differences between data sets for the unchanged evaluations are from changes in the processing of the evaluation into an MCNP data file using NJOY and *should* not be significant.

ENDF Evaluations cont.

- Isotopic evaluations for Cr, Fe, Ni, and Cu
- In the actinide region, ^{235,238}U and ^{239,241}Pu were completely updated, including an extension of the resonance region much higher in energy.
- ^{240}Pu is new relative to the ENDF/B-V data in the MCNP libraries.

ENDL92

- Received at LANL in 1995 and documented in LA-UR-96-327, “Summary Documentation for the ENDL92 Continuous-energy Neutron Data Library”
- Contains data for 106 nuclides
- LANL modified data for Zn, Sn, Pt, and Hg
- Does not have data for ^{2}H, ^{9}Be or ^{182,183,184,186}W - we will use ENDF/B-VI for these nuclides

86 k_{eff} Benchmarks in 13 Categories

- Bare spheres
- Solutions
- Water-reflected
- Polyethylene-reflected
- Be and Be-O reflected
- Graphite-reflected
- Aluminum-reflected
- Steel and Ni-reflected
- Tungsten-reflected
- Thorium-reflected
- Normal Uranium reflected
- HEU-reflected
- Other

Notes

- Benchmark specs: LA-13594 and ENDF Results: LA-13627 (on WWW)
- Errors are given at the 2σ level in the tables for k_{eff}
- ICSBEP and CSEWG specifications
- 5 benchmarks have more than one representation
  - For Flattop-23, a sphere of ^{233}U reflected by normal uranium, the CSEWG specification contains a small gap between the main fuel and the reflector, whereas the ICSBEP specification has no gap.
  - ICSBEP specifications for Godiva contain both the standard sphere of HEU as well as nested spherical shells of HEU.
  - There are two specifications for the one- and two-dimensional models for Bigten, the water-reflected sphere of HEU, and the thorium-reflected sphere of ^{239}Pu (Thor).
- There are a total of 91 MCNP input files.

Bare Spheres - ^{233,235}U and ^{239}Pu

- Think high energy (MeV)!
- ENDF Comparisons
  - ^{233}U shows little change as expected and calculates low
  - ^{238}U tends to increase k and ^{235}U tends to decrease k
    - The energy spectrum and ratio of ^{235}U to ^{238}U will determine the net effect
  - ^{239}Pu shows little change
- ENDL92
  - Overall does a bit better for fast criticals

Bare Spheres

MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2	ENDL92
23umt1	1.000±0.001	0.9942±0.0011	0.9931±0.0011	0.9974±0.0011
ieumt3	1.0000±0.0017	1.0051±0.0012	1.0005±0.0012	1.0021±0.0012
umet1ss	1.000±0.001	0.9982±0.0011	0.9963±0.0012	1.0005±0.0012
umet1ns	1.000±0.001	0.9975±0.0012	0.9968±0.0011	0.9997±0.0012
umet8	0.9989±0016	0.9942±0.0012	0.9918±0.0011	0.9948±0.0012
umet15	0.9996±0.0017	0.9931±0.0011	0.9925±0.0011	0.9957±0.0011
umet18	1.0000±0.0016	0.9984±0.0011	0.9969±0.0012	1.0012±0.0012
pumet1	1.000±0.002	0.9969±0.0012	0.9971±0.0010	0.9990±0.0011
pumet2	1.000±0.002	0.9979±0.0011	0.9992±0.0011	1.0031±0.0011
pumet22	1.0000±0.0021	0.9965±0.0011	0.9962±0.0011	0.9967±0.0012

Solution Assemblies

- Think thermal (10^{-8} MeV)!
- ENDF Comparisons
  - With no exception, there is a significant decrease in k_{eff} from B-V to B-VI data libraries.
    - bad for ^{233}U and ^{235}U solutions and good for ^{239}Pu solutions
  - New ^{1}H evaluation decreased k_{eff} by 0.0010±0.0001
  - New ^{16}O decreased k_{eff} by 0.0026±0.0002
  - No net effect due from new ^{14}N evaluation
  - New ^{239}Pu evaluation tended to decrease k_{eff} by 0.0033±0.0004 for solutions
  - New ^{235}U evaluation made very little difference
- ENDL92
  - Calculates far too high for ^{233}U and ^{239}Pu solutions (1.5-2%), and a ~0.5% high for ^{235}U solutions.

Solution Assemblies

MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2	ENDL92
23usl1a	1.0000±0.0031	1.0010±0.0007	0.9967±0.0008	1.0158±0.0007
23usl1b	1.0005±0.0033	1.0004±0.0008	0.9966±0.0008	1.0156±0.0008
23usl1c	1.0006±0.0033	0.9997±0.0008	0.9969±0.0008	1.0146±0.0008
23usl1d	0.9998±0.0033	0.9993±0.0008	0.9962±0.0008	1.0150±0.0008
23usl1e	0.9999±0.0033	0.9984±0.0008	0.9956±0.0007	1.0143±0.0008
23usl8	1.0006±0.0029	0.9987±0.0005	0.9954±0.0005	1.0109±0.0005
usol13a	1.0012±0.0026	1.0007±0.0008	0.9972±0.0007	1.0084±0.0007
usol13b	1.0007±0.0036	0.9993±0.0008	0.9964±0.0008	1.0070±0.0008
usol13c	1.0009±0.0036	0.9952±0.0009	0.9922±0.0008	1.0042±0.0008
usol13d	1.0003±0.0036	0.9981±0.0009	0.9957±0.0009	1.0055±0.0008
usol32	1.0015±0.0026	1.0003±0.0005	0.9966±0.0005	1.0036±0.0005
pnl1	1.0	1.0158±0.0013	1.0062±0.0012	1.0254±0.0013
pnl6	1.0	1.0089±0.0013	1.0020±0.0013	1.0119±0.0014
pusl11a	1.0000±0.0052	1.0019±0.0011	0.9951±0.0011	1.0128±0.0011
pusl11b	1.0000±0.0052	1.0084±0.0012	0.9998±0.0011	1.0180±0.0011
pusl11c	1.0000±0.0052	1.0137±0.0013	1.0045±0.0012	1.0226±0.0012
pusl11d	1.0000±0.0052	1.0182±0.0012	1.0085±0.0012	1.0265±0.0013

Water-Reflected Assemblies

- ENDF Comparisons
  - For the water-reflected HEU sphere, hydrogen and oxygen lowered k_{eff} and the ^{235}U evaluation increased k_{eff} - net result of no significant change
  - For the water-reflected Pu sphere, H and O lowered k_{eff}
- ENDL92 is a bit higher for water-reflected HEU sphere

MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2	ENDL92
umet4a	1.002	0.9999±0.0014	1.0010±0.0015	1.0036±0.0014
umet4b	1.0003±0.0005	0.9967±0.0015	0.9969±0.0015	0.9998±0.0014
pumet11	1.0000±0.001	1.0009±0.0014	0.9984±0.0014	0.9985±0.0015

CH_2 and Graphite-Reflected Assemblies

- ENDF Comparisons
  - Seen previously that new H evaluation tends to lower k_{eff}
  - No change in k_{eff} because of new C evaluation
  - Decrease in k_{eff} for all of the IEU assemblies due to the changes in the ^{235}U evaluation (-0.0042±0.0003)
    - Better result for graphite-reflected U assemblies though still a little high
- ENDL92 a little high for graphite-reflected U assemblies

CH_2 and Graphite-Reflected Assemblies

MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2	ENDL92
umet11	1.000±0.001	0.9924±0.0014	0.9954±0.0014	1.0000±0.0015
umet20	1.0000±0.0030	0.9958±0.0013	0.9972±0.0013	1.0005±0.0013
pumet24	1.0000±0.0020	0.9981±0.0013	1.0009±0.0012	0.9998±0.0012
ieumt4	1.0000±0.0030	1.0091±0.0012	1.0051±0.0012	1.0065±0.0012
umet19	1.0000±0.0030	1.0040±0.0012	1.0031±0.0012	1.0077±0.0012
pumet23	1.0000±0.0020	0.9973±0.0012	0.9973±0.0012	1.0010±0.0012

Be and BeO-Reflected Assemblies

- ENDF Comparisons
  - Sensitivity studies show that changes in the new Be evaluation do not significantly affect the calculations
  - the new ^{16}O evaluation lowers k_{eff} by 0.0039 ± 0.0006 for the two BeO benchmarks
- *ENDL92 results use the ENDF/B-VI data for Be.*

Be and BeO-Reflected Assemblies

MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2	ENDL92
23umt5a	1.0000±0.0030	0.9940±0.0012	0.9962±0.0012	0.9984±0.0012
23umt5b	1.0000±0.0030	0.9955±0.0013	0.9967±0.0014	1.0016±0.0013
umet9a	0.9992±0.0015	0.9927±0.0012	0.9958±0.0012	0.9952±0.0012
umet9b*	0.9992±0.0015	0.9962±0.0012	0.9936±0.0012	0.9975±0.0012
pumet18	1.0000±0.0030	0.9999±0.0013	0.9999±0.0012	0.9978±0.0013
pumet19	0.9992±0.0015	1.0016±0.0013	1.0032±0.0012	0.9986±0.0013
pumt21a	1.0000±0.0026	1.0033±0.0013	1.0042±0.0013	1.0021±0.0013
pumt21b*	1.0000±0.0026	0.9970±0.0012	0.9945±0.0012	0.9961±0.0013

With a different initial random number, the differences for 23umt5a and umet9a disappear.

MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2
23umt5a	1.0000±0.0030	0.9940±0.0012	0.9941±0.0012
umet9a	0.9992±0.0015	0.9927±0.0012	0.9958±0.0012

Aluminum-Reflected Assemblies

- ENDF Comparisons
  - No change in the Al evaluation between B-V and B-VI
  - The largest change in k_{eff} is for *ieumt6*, which shows a decrease similar to that seen for the other IEU assemblies from ^{235}U
- ENDL92 shows similar results to ENDF

MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2	ENDL92
ieumt6	1.0000±0.0023	0.9964±0.0012	0.9917±0.0012	0.9912±0.0011
umet12	0.9992±0.0018	0.9932±0.0011	0.9941±0.0012	0.9935±0.0012
umet22	1.0000±0.0021	0.9919±0.0012	0.9924±0.0012	0.9943±0.0012
pumet9	1.0000±0.0027	1.0003±0.0012	1.0022±0.0011	1.0007±0.0011

Steel and Ni-Reflected Assemblies

- ENDF Comparisons
  - New isotopic evaluations for of Cr, Fe, Ni, and Cu
  - The steel-reflected assemblies show a consistent decrease in k_{eff} from B-V to B-VI data. Sensitivity studies showed that there was an average decrease in k_{eff} for iron of 0.0048±0.0006 for these benchmarks
  - For Ni, studies indicated that the new evaluations decreased k_{eff} by 0.0104±0.0014, moving it closer to the benchmark value
- ENDL92 results for steel-reflected assemblies are quite high (proportional to size of reflector).

Steel and Ni-Reflected Assemblies

MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2	ENDL92
ieumt5 - 8.25 cm	1.0000±0.0021	1.0112±0.0011	1.0007±0.0012	1.0403±0.0013
umet13 - 3.65 cm	0.9990±0.0015	0.9982±0.0012	0.9941±0.0013	1.0103±0.0012
umet21- 9.7 cm	1.0000±0.0026	1.0023±0.0012	0.9947±0.0012	1.0390±0.0013
pumet25 - 1.55 cm	1.0000±0.0020	0.9984±0.0012	0.9963±0.0012	0.9960±0.0012
pumet26- 11.9 cm	1.0000±0.0024	1.0016±0.0012	0.9971±0.0012	1.0320±0.0013
umet3l - 20.32 cm	1.0000±0.0030	1.0148±0.0013	1.0049±0.0012	1.0061±0.0013

Tungsten-Reflected Assemblies

- ENDF Comparisons
  - The evaluations for tungsten isotopes are equivalent for B-V (.55c) and B-VI (.60c) data.
  - k_{eff} is running slightly high for all benchmarks, and more so for the thickest W-reflected U and the Pu assembly.
  - Only *umet3h* shows a significant change in k_{eff}. We ran the B-VI version of this benchmark using a different starting random number. The result was a k_{eff} of 1.0049±0.0006, indicating that the drop in k_{eff} was a statistical fluctuation.
- ENDL92 results use ENDF/B-VI data for W isotopes.

W-Reflected Assemblies

MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2	ENDL92
23umt4a - 2.44 cm	1.0000±0.0007	1.0037±0.0012	1.0031±0.0012	1.0039±0.0012
23umt4b - 5.79 cm	1.0000±0.0008	1.0059±0.0013	1.0049±0.0012	1.0071±0.0013
umet3h - 4.83 cm	1.0000±0.0050	1.0055±0.0013	1.0065±0.0013	1.0066±0.0011
umet3i - 7.37 cm	1.0000±0.0050	1.0053±0.0012	1.0066±0.0013	1.0073±0.0012
umet3j - 11.43 cm	1.0000±0.0050	1.0056±0.0012	1.0068±0.0013	1.0072±0.0012
umet3k - 16.51 cm	1.0000±0.0050	1.0089±0.0012	1.0094±0.0014	1.0091±0.0012
pumet5 - 4.70 cm	1.0000±0.0013	1.0080±0.0013	1.0102±0.0012	1.0047±0.0012

Thorium-Reflected Assemblies

- There are 1D and 2D representations of Thor
- ENDF Comparisons
  - No change in evaluation for ^{232}Th
  - The slight increase in k_{eff} follows the same pattern that we have seen for the Jezebel and Jezebel-Pu assemblies (pumet1 and pumet2).
- ENDL92 closer to benchmark values.

MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2	ENDL92
pumet8a	1.0000±0.0030	1.0042±0.0012	1.0064±0.0012	0.9992±0.0011
pumet8b	1.000±0.0006	1.0045±0.0013	1.0072±0.0012	1.0004±0.0012

Normal Uranium Reflected Assemblies

- ENDF Comparisons
  - Half of the assemblies show a change in the calculated k_{eff} of more than 2σ.
  - Changes in both the ^{235}U and ^{238}U evaluations have competing effects.
  - On average, the change in the ^{235}U evaluation caused a decrease in k_{eff} of 0.0022 ± 0.0002, while the changes in the ^{238}U evaluation caused an increase in k_{eff} of 0.0012 ± 0.0002
- ENDL92 calculates quite low for Bigten assembly.

U(N)-Reflected Assemblies

MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2	ENDL92
23umt3a	1.0000±0.0010	0.9974±0.0011	0.9971±0.0011	1.0017±0.0012
23umt3b	1.0000±0.0010	0.9983±0.0012	0.9991±0.0012	1.0051±0.0012
23umt6	1.0000±0.0014	0.9992±0.0013	0.9997±0.0014	1.0012±0.0014
flat23	1.000±0.001	1.0030±0.0013	1.0034±0.0013	1.0035±0.0013
ieumt2	1.000±0.003	1.0081±0.0011	1.0034±0.0011	0.9947±0.0011
umet3a	1.0000±0.0050	0.9954±0.0012	0.9920±0.0012	0.9944±0.0012
umet3b	1.0000±0.0050	0.9956±0.0012	0.9936±0.0012	0.9950±0.0013
umet3c	1.0000±0.0050	1.0006±0.0013	0.9979±0.0013	0.9969±0.0011
umet3d	1.0000±0.0030	0.9984±0.0012	0.9950±0.0012	0.9964±0.0013
umet3e	1.0000±0.0030	1.0029±0.0012	1.0014±0.0013	0.9982±0.0013
umet3f	1.0000±0.0030	1.0018±0.0012	1.0006±0.0013	0.9970±0.0013
umet3g	1.0000±0.0030	1.0039±0.0013	1.0019±0.0013	0.9964±0.0012
umet14	0.9989±0.0017	0.9972±0.0013	0.9957±0.0012	0.9971±0.0012
umet28	1.0000±0.0030	1.0030±0.0012	1.0027±0.0013	0.9995±0.0013
bigten1	0.996±0.003	1.0059±0.0010	1.0069±0.0010	0.9831±0.0010
bigten2	0.996±0.003	1.0035±0.0009	1.0045±0.0009	0.9808±0.0009
pumet6	1.0000±0.0030	1.0039±0.0013	1.0040±0.0014	1.0008±0.0013
pumet10	1.0000±0.0018	0.9984±0.0012	1.0005±0.0012	1.0018±0.0012
pumet20	0.9993±0.0017	0.9998±0.0012	0.9997±0.0013	1.0008±0.0012

HEU-Reflected Assemblies

- The first two benchmarks, *23umt2a* and *23umt2b*, have a ^{233}U core, while *mixmet1* and *mixmet3* have a ^{239}Pu core.
- ENDF Comparisons
  - ^{233}U did not change from B-V to B-VI.
  - The larger the HEU reflector, the larger the decrease in k_{eff}.
- ENDL92 consistently calculates higher than ENDF for these benchmarks - usually closer to benchmark.

MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2	ENDL92
23umt2a	1.0000±0.0010	0.9952±0.0011	0.9961±0.0011	1.0017±0.0012
23umt2b	1.0000±0.0011	0.9991±0.0011	0.9968±0.0011	1.0037±0.0012
mixmet1	1.0000±0.0016	0.9966±0.0012	0.9969±0.0012	0.9993±0.0011
mixmet3	0.9993±0.0016	1.0000±0.0012	0.9979±0.0012	1.0008±0.0013

Other Assemblies

- The *ieumt1* (Jemima) series of benchmarks are cylindrical disks of HEU and normal uranium. The MCNP model is slightly idealized, but still maintains the heterogeneous description of the disks. It has been shown that performing a criticality calculation using a homogenous material gives too large a discrepancy in k_{eff}.
- ENDF
  - The changes to the ^{235}U evaluation tend to decrease k_{eff} for the Jemima assemblies (-0.0032±0.0004), and are greater than changes in k_{eff} due the new ^{238}U evaluation.

Other Assemblies Cont.

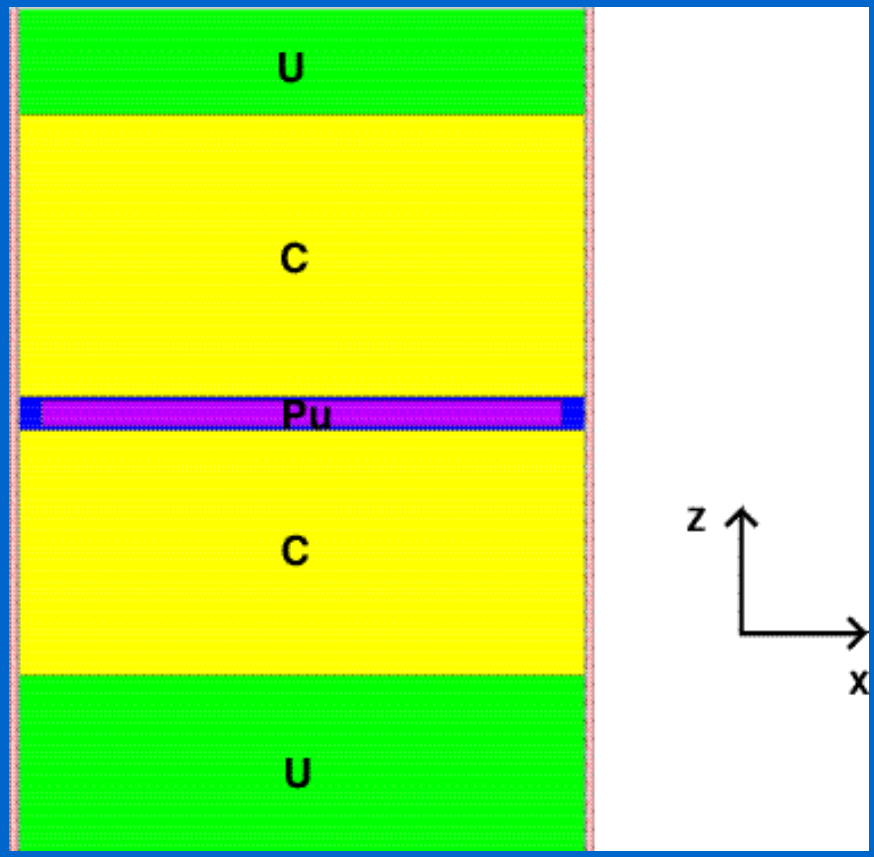
- The *mixmet8* assembly is a rectangular graphite- and normal uranium-reflected slab of ^{239}Pu
- There is a large discrepancy in the mixmet8 calculations from ^{238}U.
- ENDF: Sensitivity tests showed that there was little effect from the new evaluations for ^{235}U, ^{239}Pu, and $^{54,56,57,58}Fe$, but that the ^{238}U evaluation increased k_{eff} by 0.0265±0.0007.
- Improvements to the data through the resonance region substantially improve the ^{238}U evaluation.

Other Critical Assemblies

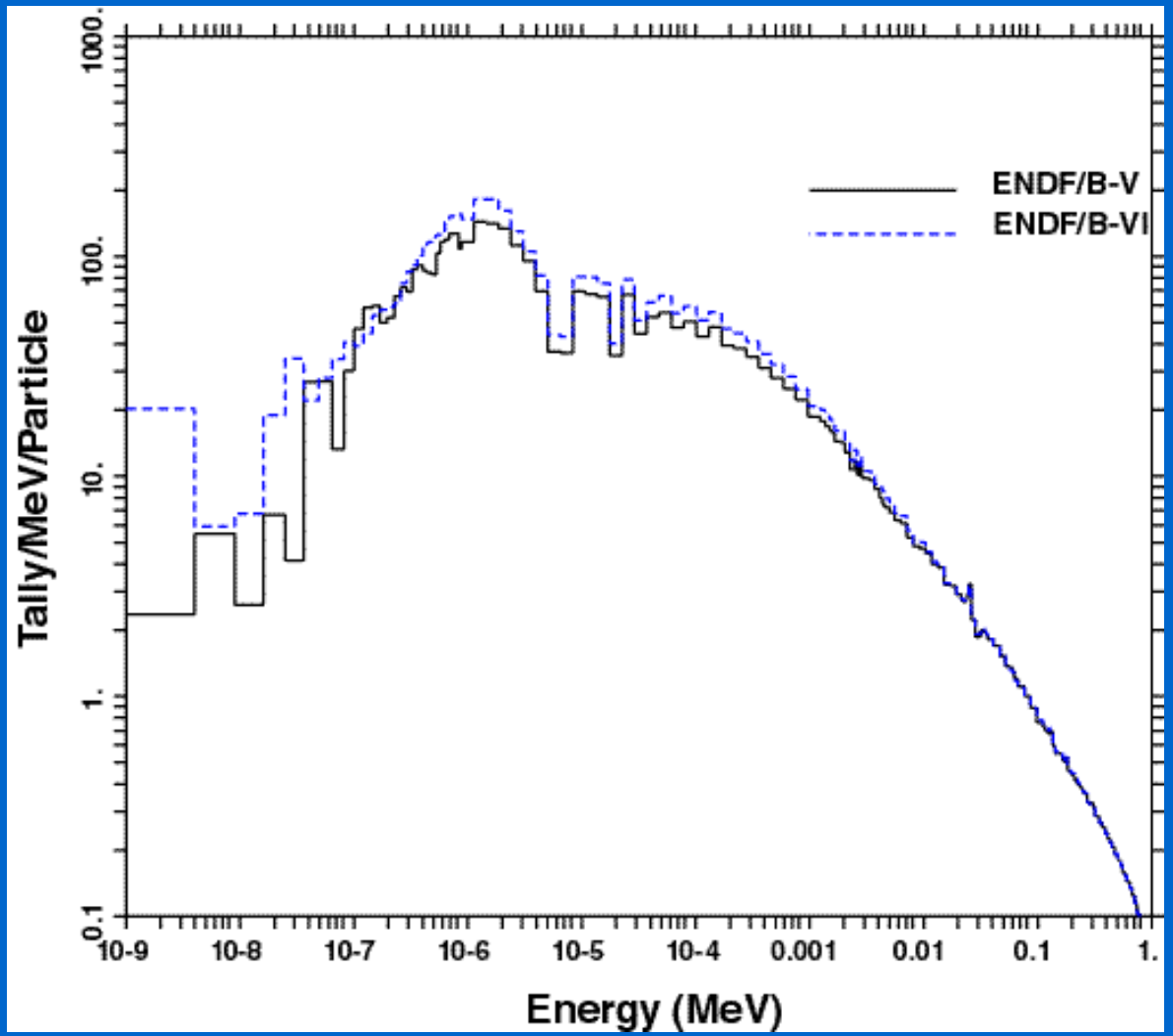
MCNP Filename	Benchmark	ENDF/B-V	ENDF/B-VI R2	ENDL92
mixmet8	0.9920±0.0063	0.9591±0.0009	0.9918±0.0010	0.8690±0.0008
ieumt1a	0.9989	1.0024±0.0012	0.9961±0.0012	0.9988±0.0012
ieumt1b	0.9997	1.0018±0.0012	0.9974±0.0012	1.0006±0.0012
ieumt1c	0.9993	1.0035±0.0012	0.9988±0.0012	1.0007±0.0011
ieumt1d	1.0002	1.0039±0.0012	0.9984±0.0012	1.0010±0.0012

mixmet8 MCNP Geometry

- k_∞ benchmark
- Graphite (C) and normal-uranium(U) reflected Pu slab.
- The outer surfaces of the MCNP geometry in the figure are periodic. The outer surface normal to the y-axis, which is not shown, is reflective.



Neutron Flux in U-reflector of *mixmet8*



k_{eff} Summary (1)

- Fast Systems
  - ENDF ^{233}U unchanged and calculates low (0.5%)
  - New ENDF/B-VI R2 evaluations for ^{235}U tends to increase k_{eff} while the new ^{238}U tends to decreases k_{eff}
    - Energy spectrum and ratio of ^{235}U to ^{238}U determines net effect
  - ^{239}Pu shows a very slight increase
  - ENDL92 calculates fast critical assemblies a bit better than ENDF

k_{eff} Summary (2)

- Thermal systems
  - New ENDF for ^{1}H and ^{16}O decrease k_{eff} by 0.1% and 0.26% respectively
  - New ENDF ^{14}N and ^{235}U have no effect
  - New ENDF ^{239}Pu decreases k_{eff} by 0.33%
  - ENDL92 calculates very high (avg. 1.4%)
  - Important to use proper S(α,β) data for thermal upscatter (water, poly, …)

k_{eff} Summary (3)

- New ENDF carbon shows no effect for CH_2 and graphite-reflected systems, while ENDL92 calculates high (1%) for graphite-reflected U systems
  - New ENDF H tends to lower k_{eff}
- New ENDF ^{9}Be evaluation does not impact k_{eff}, but new ^{16}O decreases k_{eff} by 0.4% for BeO-reflected systems
- New ENDF isotopic evaluations for Fe and Ni decrease k_{eff} by 0.5% and 1% respectively. For Ni this greatly improves the calculated k_{eff}.
- ENDL92 calculates very high, 2.3% for Fe and 0.6% for Ni.

k_{eff} Summary (4)

- No significant differences between libraries for Al-reflected assemblies, ~0.5% low
- No significant differences between ENDF libraries for W-reflected assemblies, ~0.6% high
- ENDF Th-reflected assembly is ~0.5% high, while ENDL92 is close to 1.0
- New ENDF evaluation for ^{238}U significantly improves the mixed-metal assembly (mixmet8), ENDL92 does a very poorly (~13% low)