LA-UR-11-06327

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Title:	MCNP Results for ENDF/B-VII.1beta4
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Intended for:	2011 Annual CSEWG Meeting Brookhaven National Laboratory November 15 - 17, 2011

Form 836 (7/06)

MCNP Results for ENDF/B-VII.1β4

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Presented at the 2011 CSEWG Meeting
Brookhaven National Laboratory November 15-17, 2011

Results obtained with the MCNP Monte Carlo code and the ENDF/B-VII.1β4 nuclear data library are presented for a variety of benchmarks. Those results are compared with results for the same benchmarks obtained with MCNP and the ENDF/B-VII.0 nuclear data library.

Significant improvements are found for benchmarks that contain beryllium, cadmium, or tungsten, and some improvement for benchmarks with zirconium also is seen. The results for the benchmarks with beryllium suggest that further improvements still may be needed. The other benchmarks studied show only relatively minor or negligible changes.

A number of deficiencies previously identified for the ENDF/B-VII.0 library still remain for ENDF/B-VII.1β4. Those deficiencies include ^{235}U cross sections in the unresolved resonance range, thermal cross sections for ^{239}Pu, and fast cross sections for copper, ^{237}Np, and ^{232}Th.

MCNP Results for ENDF/B-VII.1β4

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Overview of Presentation

Little if any change in results for for most cases in the expanded criticality validation suite for MCNP (e.g., metal spheres)

Improved results for benchmarks with tungsten, beryllium, cadmium, or zirconium

Results from some additional benchmarks with unresolved problems

Results for cases in the Rossi α validation suite

Summary and conclusions

Expanded Criticality Validation Suite for MCNP

Principal Fuel	Number of Benchmarks by Spectrum			
	Fast	Intermediate	Thermal	Total
^{233}U	10	1	7	18
HEU	29	5	6	40
IEU	10	1	6	17
LEU			8	8
Plutonium	21	1	14	36
Total	70	8	41	119

Calculations were performed for all of these benchmarks as well as several additional benchmarks

All benchmark specifications are taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*

Results for HEU Spheres

Reflector	Benchmark k_{eff}	MCNP5 k_{eff}	
		ENDF/B-VII.1β4	ENDF/B-VII.0
None	1.0000 ± 0.0010	0.9997 ± 0.0003	0.9994 ± 0.0003
None	1.0000 ± 0.0014	0.9996 ± 0.0003	0.9999 ± 0.0003
Normal U	1.0000 ± 0.0050	0.9948 ± 0.0003	0.9948 ± 0.0003
Normal U	1.0000 ± 0.0050	0.9946 ± 0.0003	0.9945 ± 0.0003
Normal U	1.0000 ± 0.0050	0.9993 ± 0.0003	0.9991 ± 0.0003
Normal U	1.0000 ± 0.0030	0.9970 ± 0.0003	0.9971 ± 0.0003
Normal U	1.0000 ± 0.0030	1.0014 ± 0.0003	1.0008 ± 0.0003
Normal U	1.0000 ± 0.0030	1.0018 ± 0.0003	1.0020 ± 0.0003
Normal U	1.0000 ± 0.0030	1.0024 ± 0.0003	1.0018 ± 0.0003
Depleted U	0.9989 ± 0.0017	0.9975 ± 0.0003	0.9978 ± 0.0003

$\sigma < |\Delta k| \leq 2\sigma$

Results for Plutonium Spheres

Reflector	Benchmark k_{eff}	MCNP5 k_{eff}	
		ENDF/B-VII.1β4	ENDF/B-VII.0
None	1.0000 ± 0.0010	1.0000 ± 0.0003	1.0000 ± 0.0003
None	1.0000 ± 0.0014	1.0000 ± 0.0003	0.9999 ± 0.0003
Normal U	1.0000 ± 0.0030	1.0000 ± 0.0003	0.9995 ± 0.0003
Normal U	1.0000 ± 0.0018	0.9990 ± 0.0003	1.0001 ± 0.0003
Depleted U	0.9993 ± 0.0017	0.9981 ± 0.0003	0.9981 ± 0.0003
Thorium	1.0000 ± 0.0006	0.9978 ± 0.0003	0.9977 ± 0.0003

$|\Delta k| > 3\sigma$

For the last case (Thor), less than 6% of the fissions occur in the thorium reflector

Results for ^{233}U Spheres

Reflector	Benchmark k_{eff}	MCNP5 k_{eff}	
		ENDF/B-VII.1β4	ENDF/B-VII.0
None	1.0000 ± 0.0010	0.9998 ± 0.0003	0.9995 ± 0.0003
HEU	1.0000 ± 0.0010	0.9988 ± 0.0003	0.9990 ± 0.0003
HEU	1.0000 ± 0.0011	1.0005 ± 0.0003	1.0006 ± 0.0003
Normal U	1.0000 ± 0.0010	0.9992 ± 0.0003	0.9996 ± 0.0003
Normal U	1.0000 ± 0.0010	0.9997 ± 0.0003	1.0001 ± 0.0003
Normal U	1.0000 ± 0.0014	0.9985 ± 0.0003	0.9995 ± 0.0003

$\sigma < |\Delta k| \leq 2\sigma$

Results for Metal Spheres Reflected by Tungsten or Tungsten Carbide

Fuel	Fuel Radius (cm)	Reflector Thickness (cm)	Benchmark k_{eff}	MCNP5 k_{eff}	
				ENDF/B-VII.1β4	ENDF/B-VII.0
^{233}U	5.0444	2.4384	1.0000 ± 0.0007	0.9984 ± 0.0003	1.0049 ± 0.0003
^{233}U	4.5999	5.7912	1.0000 ± 0.0008	0.9955 ± 0.0003	1.0052 ± 0.0003
HEU	6.6020	4.8260*	1.0000 ± 0.0050	1.0016 ± 0.0003	1.0082 ± 0.0003
HEU	6.2527	7.3660*	1.0000 ± 0.0050	1.0014 ± 0.0003	1.0095 ± 0.0003
HEU	6.0509	11.4300*	1.0000 ± 0.0050	1.0051± 0.0003	1.0129 ± 0.0003
HEU	6.0159	16.5100*	1.0000 ± 0.0050	1.0097 ± 0.0003	1.0166 ± 0.0003
Pu	5.0419	4.6990	1.0000 ± 0.0013	1.0008 ± 0.0003	1.0093 ± 0.0003

* Tungsten carbide reflector $\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$

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Results for Metal Spheres Reflected by Beryllium or Beryllium Oxide

Fuel	Fuel Radius (cm)	Reflector Thickness (cm)	Benchmark k_{eff}	MCNP5 k_{eff}	
				ENDF/B-VII.1β4	ENDF/B-VII.0
^{233}U	5.0444	2.0447	1.0000 ± 0.0030	0.9964 ± 0.0003	0.9941 ± 0.0003
^{233}U	4.5999	4.1961	1.0000 ± 0.0030	0.9956 ± 0.0003	0.9924 ± 0.0003
HEU	8.3500	2.6500	0.9992 ± 0.0015	0.9979 ± 0.0003	0.9949 ± 0.0003
HEU	8.3500*	2.6500**	0.9992 ± 0.0015	0.9965 ± 0.0003	0.9955 ± 0.0003
Pu	5.0419	3.6881	1.0000 ± 0.0030	0.9997 ± 0.0003	0.9964 ± 0.0003

* Inner radius 1.4 cm
** Beryllium oxide reflector

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$

All of these benchmarks are extrapolated from **subcritical** experiments with low multiplication (400 maximum, some less than 100)

Results for Metal Spheres and Cylinders Reflected by Beryllium or Beryllium Oxide

Fuel	Fuel Radius / Height (cm)	Reflector Radius / Height (cm)	Benchmark k_{eff}	MCNP5 k_{eff}	
				ENDF/B-VII.1β4	ENDF/B-VII.0
Pu	5.9950 / 4.5000	9.9950 / 14.8950	1.0000 ± 0.0026	1.0046 ± 0.0003	1.0031 ± 0.0003
Pu	5.9950 / 4.5000	9.9950 / 14.9400**	1.0000 ± 0.0026	0.9930 ± 0.0003	0.9929 ± 0.0003
Pu	5.3500*	5.6500	0.9992 ± 0.0015	1.0009 ± 0.0003	0.9976 ± 0.0003
Pu	3.7938	8.4938	0.9983 ± 0.0019	1.0000 ± 0.0003	0.9965 ± 0.0003

* Inner radius 1.4 cm
** Beryllium oxide reflector

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$

All of these benchmarks are based on **critical** experiments

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Results for Water-Moderated LWBR SB Cores

Case	Fuel	Lattice	Benchmark k_{eff}	MCNP5 k_{eff}	
				ENDF/B-VII.1β4	ENDF/B-VII.0
SB-1	$^{235}UO_2$-ZrO_2	Rect	1.0006 ± 0.0027	0.9995 ± 0.0004	1.0017 ± 0.0004
SB-5	$^{235}UO_2$-ZrO_2	Hex	1.0015 ± 0.0028	0.9986 ± 0.0004	0.9999 ± 0.0004
SB-2	$^{233}UO_2$-ZrO_2	Rect	1.0015 ± 0.0025	1.0021 ± 0.0005	1.0043 ± 0.0005
SB-2½	$^{233}UO_2$-ZrO_2	Rect	1.0000 ± 0.0024	1.0019 ± 0.0005	1.0044 ± 0.0005
SB-6	$^{233}UO_2$-ZrO_2	Hex	0.9995 ± 0.0027	1.0018 ± 0.0004	1.0032 ± 0.0004

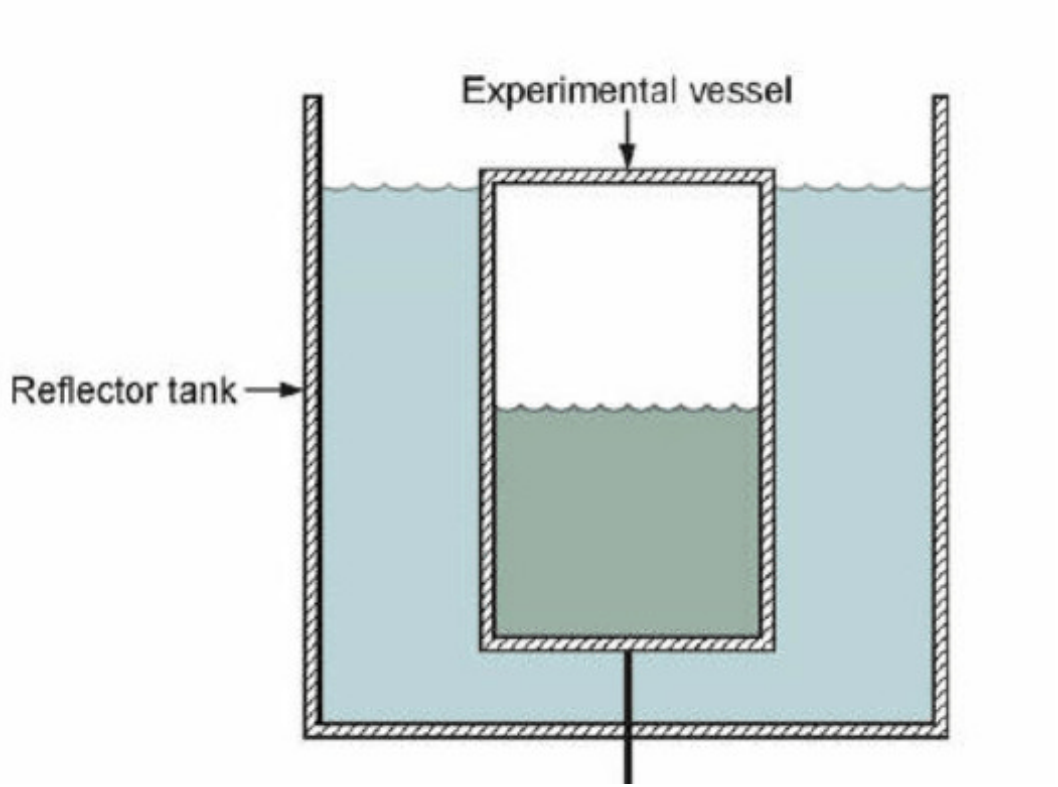
$\sigma < |\Delta k| \leq 2\sigma$

All cores except SB-2½ are surrounded by a blanket of ThO_2 pins in water

The SB-2½ core is surrounded by a water reflector

Improvement is due to changes in zirconium data in going from ENDF/B-VII.1β3 to ENDF/B-VII.1β4

Simplified Diagram of the Experiments with HEU Solutions Containing Cadmium



Results for HEU Solutions with Cadmium (Smaller Vessel)

Case	In-Vessel Cd Conc. (mg/g)	Benchmark k_{eff}	Calculated k_{eff}	
			ENDF/B-VII.1β4	ENDF/B-VII.0
1	0	1.0012 ± 0.0026	0.9989 ± 0.0004	0.9997 ± 0.0004
2*	0	1.0012 ± 0.0029	0.9908 ± 0.0004	0.9897 ± 0.0004
3	1.208	1.0012 ± 0.0026	0.9981 ± 0.0004	0.9957 ± 0.0004
4	2.393	1.0012 ± 0.0025	0.9996 ± 0.0004	0.9955 ± 0.0004
5	3.897	1.0012 ± 0.0025	1.0029 ± 0.0004	0.9974 ± 0.0004
6	4.069	1.0012 ± 0.0025	1.0047 ± 0.0004	0.9998 ± 0.0004
7	4.196	1.0012 ± 0.0024	1.0051 ± 0.0004	0.9995 ± 0.0004
8	4.271	1.0012 ± 0.0024	1.0041 ± 0.0004	0.9983 ± 0.0004

* Reflector contains Cd $\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$

Results for HEU Solutions with Cadmium (Larger Vessel)

Case	In-Vessel Cd Conc. (mg/g)	Benchmark k_{eff}	Calculated k_{eff}	
			ENDF/B-VII.1β4	ENDF/B-VII.0
9	0	1.0012 ± 0.0020	0.9976 ± 0.0004	0.9980 ± 0.0004
10*	0	1.0012 ± 0.0024	0.9894 ± 0.0004	0.9892 ± 0.0004
11*	1.240	1.0012 ± 0.0022	0.9919 ± 0.0004	0.9895 ± 0.0004
12*	2.250	1.0012 ± 0.0021	0.9957 ± 0.0004	0.9920 ± 0.0004
13*	3.362	1.0012 ± 0.0021	1.0072 ± 0.0004	0.9915 ± 0.0004
14*	4.189	1.0012 ± 0.0020	1.0082 ± 0.0004	0.9919 ± 0.0004
15*	4.577	1.0012 ± 0.0021	1.0002 ± 0.0004	0.9943 ± 0.0004
16*	4.897	1.0012 ± 0.0020	0.9993 ± 0.0004	0.9920 ± 0.0004
17*	5.047	1.0012 ± 0.0021	0.9977 ± 0.0004	0.9909 ± 0.0004
18	5.032	1.0012 ± 0.0020	0.9995 ± 0.0004	0.9933 ± 0.0004
19	5.937	1.0012 ± 0.0020	1.0006 ± 0.0004	0.9936 ± 0.0004
20	6.626	1.0012 ± 0.0019	0.9989 ± 0.0004	0.9913 ± 0.0004

* Reflector contains Cd $\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$

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Results for Water-Reflected Plutonium-Nitrate Solutions (42.9 wt.% ^{240}Pu, 1.08 wt.% ^{241}Am, 0.0089 wt.% Gd)

Pu Conc (g/liter)	Benchmark k_{eff}	MCNP5 k_{eff}		Δk VII.1β4 - VII.0
		ENDF/B-VII.1β4	ENDF/B-VII.0	
140.0	1.0000 ± 0.0034	1.0089 ± 0.0004	1.0089 ± 0.0004	0 ± 0.0006
116.0	1.0000 ± 0.0034	1.0116 ± 0.0004	1.0124 ± 0.0004	**-.0008 ± 0.0006**
99.3	1.0000 ± 0.0032	1.0098 ± 0.0004	1.0098 ± 0.0004	0 ± 0.0006
85.5	1.0000 ± 0.0030	1.0081 ± 0.0004	1.0083 ± 0.0004	-.0002 ± 0.0006
75.6	1.0000 ± 0.0030	1.0074 ± 0.0004	1.0077 ± 0.0004	-.0003 ± 0.0006
65.1	1.0000 ± 0.0031	1.0053 ± 0.0004	1.0058 ± 0.0004	-.0005 ± 0.0006
56.3	1.0000 ± 0.0032	1.0043 ± 0.0004	1.0048 ± 0.0004	-.0005 ± 0.0006
46.8	1.0000 ± 0.0033	1.0041 ± 0.0004	1.0043 ± 0.0004	-.0002 ± 0.0006
40.6	1.0000 ± 0.0034	1.0026 ± 0.0003	1.0030 ± 0.0003	-.0004 ± 0.0004

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$ **$\sigma < |\Delta k|$**

Change in ^{157}Gd data slightly reduces the calculated k_{eff} for ENDF/B-VII.1β4

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Results for Spheres Reflected by Graphite

Fuel	Fuel Radius (cm)	Reflector Thickness (cm)	k_{eff}		
			Benchmark	ENDF/B-VII.1β4	ENDF/B-VII.0
HEU	9.15*	3.45	1.0000 ± 0.0028	1.0075 ± 0.0003	1.0072 ± 0.0003
IEU	14.00**	3.20	1.0000 ± 0.0030	1.0073 ± 0.0003	1.0075 ± 0.0003
Pu	6.00***	5.65	1.0000 ± 0.0020	0.9999 ± 0.0003	0.9998 ± 0.0003

* Inner radius 4.029 cm
** Inner radius 2.788 cm
*** Inner radius 1.715 cm

$2\sigma < |\Delta k| \leq 3\sigma$

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Results for HEU Sphere Reflected by Nickel

Fuel Radius (cm)	Reflector Thickness (cm)	k_{eff}		
		Benchmark	ENDF/B-VII.1β4	ENDF/B-VII.0
6.46	26.78	1.0000 ± 0.0030	1.0084 ± 0.0003	1.0083 ± 0.0003

$2\sigma < |\Delta k| \leq 3\sigma$

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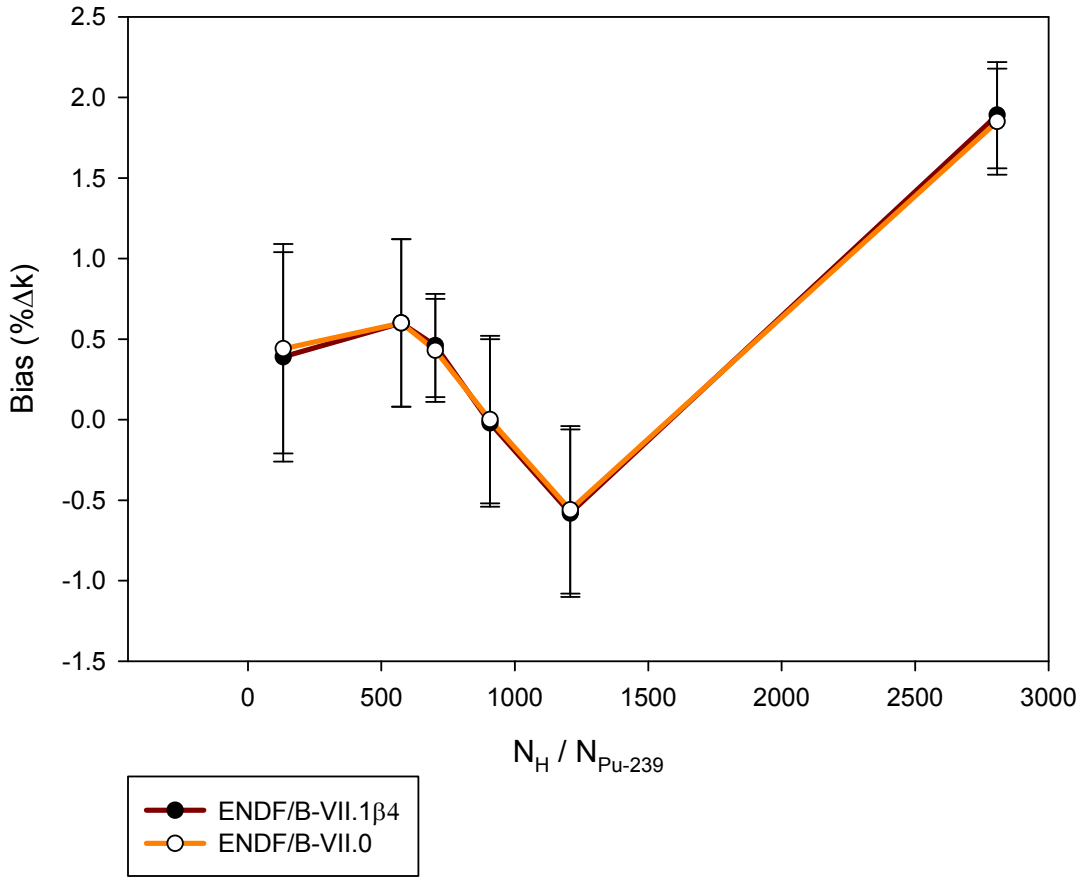
Reactivity Biases for Plutonium Solution Benchmarks



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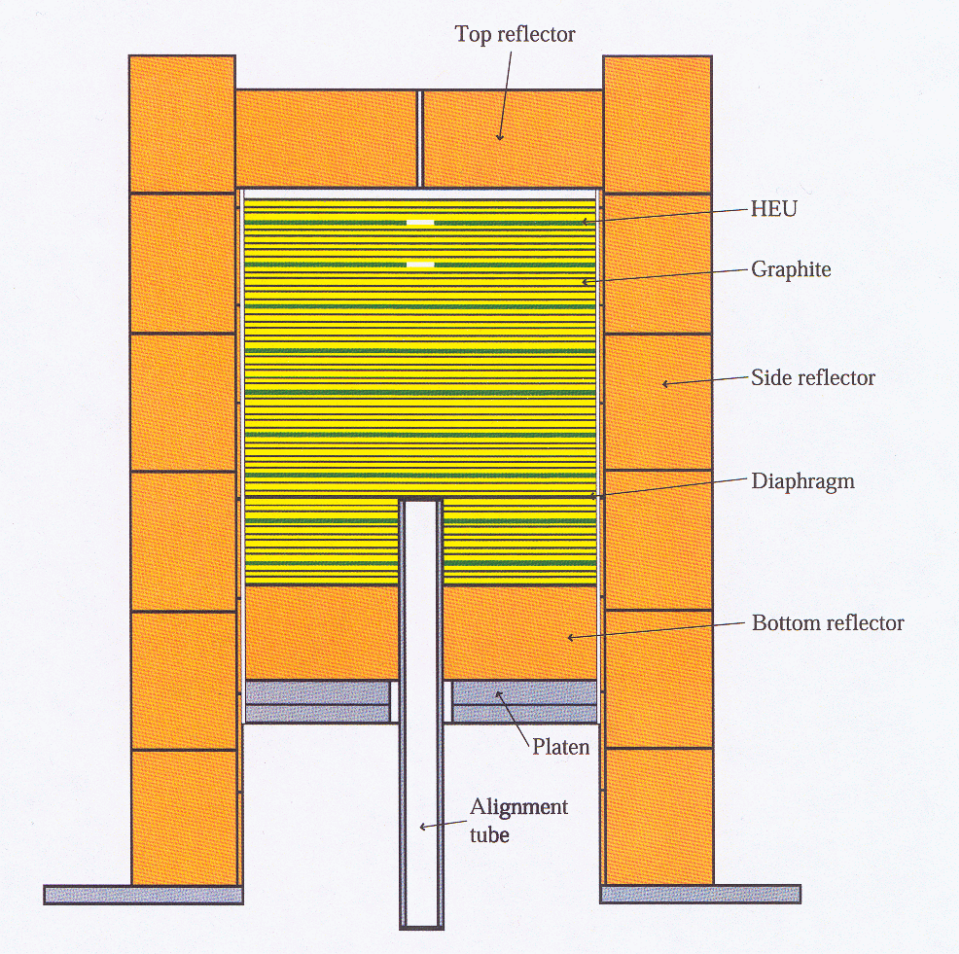
Configuration for the Zeus Benchmarks



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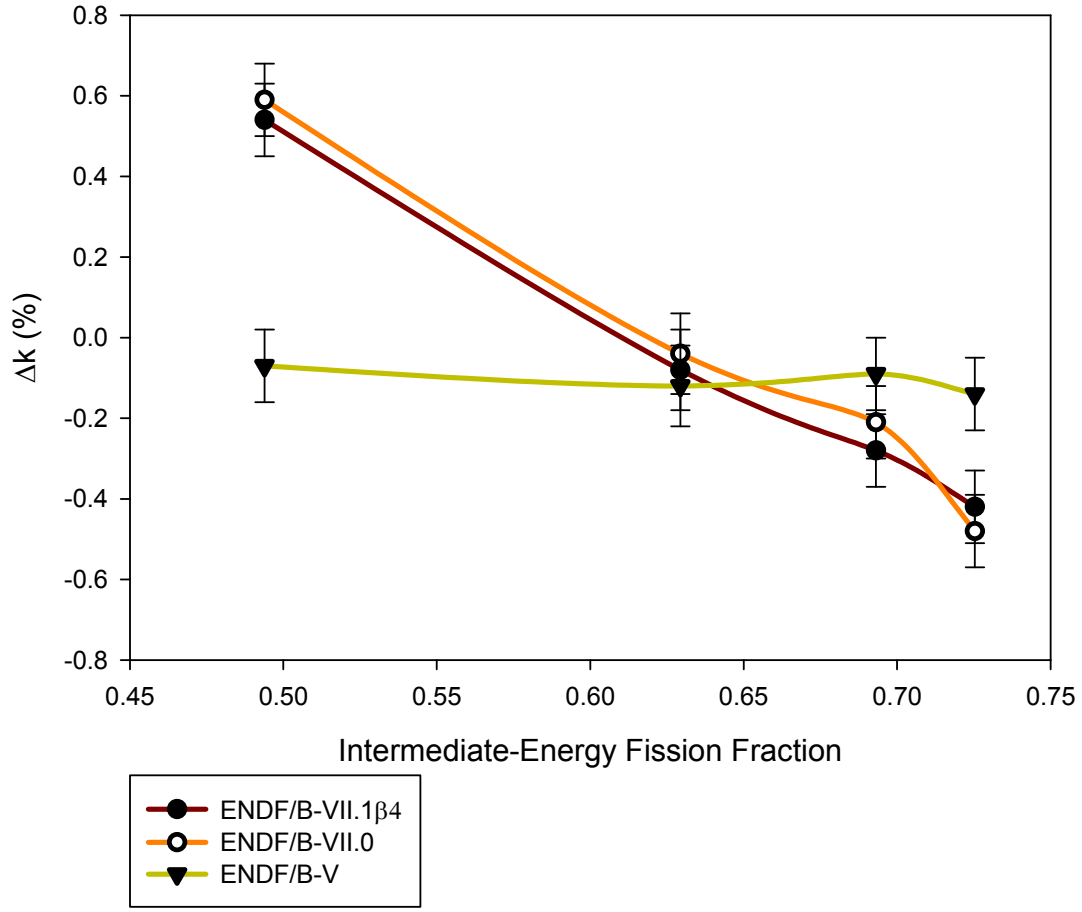
Results for the Zeus Graphite Benchmarks



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Results for the Fast Zeus Benchmarks

Moderator	Benchmark k_{eff}	MCNP5 k_{eff}		
		ENDF/B-VII.1β4 + ENDF/B-V Cu	ENDF/B-VII.1β4	ENDF/B-VII.0
Steel	0.9991 ± 0.0024	0.9998 ± 0.0003	1.0091 ± 0.0003	1.0090 ± 0.0003
None	1.0004 ± 0.0016	1.0000 ± 0.0003	1.0115 ± 0.0003	1.0115 ± 0.0003

$4\sigma < |\Delta k| \leq 5\sigma$ $6\sigma < |\Delta k| \leq 7\sigma$

ENDF/B-VII.1β4 data for copper are unchanged from the ENDF/B-VII.0 data

Replacing ENDF/B-VII copper data with ENDF/B-V data produces excellent agreement with benchmark values

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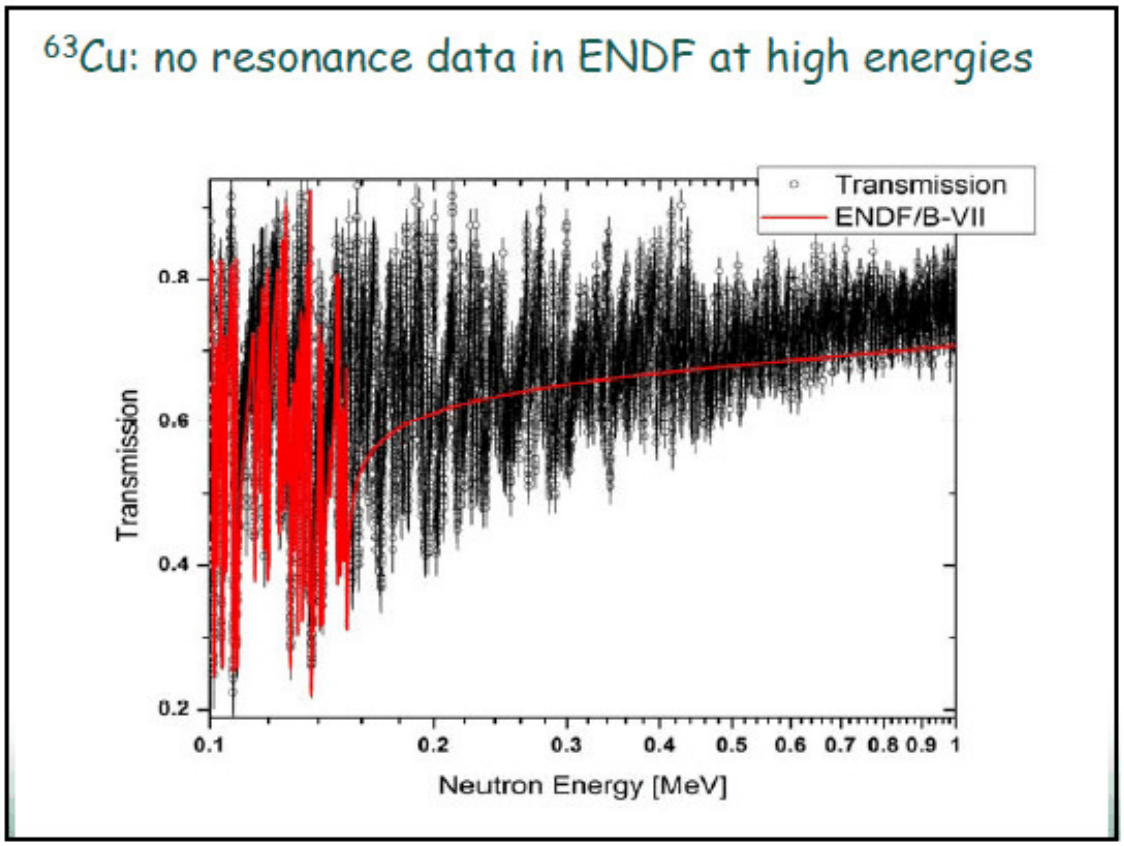
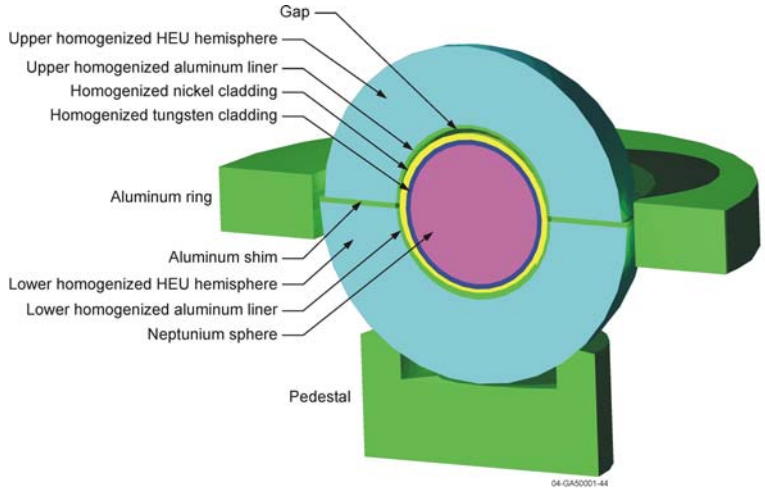
Transmission Measurements for ^{63}Cu at GELINA



K. Guber, L. Leal, C. Lampoudis, S. Kopecky, P. Schillebeeckx, F. Emiliani, R. Wynants, and P. Siegler, "New Improved Nuclear Data for Nuclear Criticality and Safety," *Proceedings of the International Conference on Nuclear Criticality 2011*, Edinburgh, Scotland (September 19-22, 2011).

Results for Neptunium Sphere Reflected by HEU



k_{eff}		
Benchmark	ENDF/B-VII.1β4	ENDF/B-VII.0
1.0019 0.0036	0.9948 ± 0.0003	0.9955 ± 0.0003

$\sigma < |\Delta k| \leq 2\sigma$

Only about 1 fission in 8 occurs in ^{237}Np

Rossi α

Rossi α is the rate of change of the population of prompt neutrons that cause fission:

$$\varphi_{pf}(t) = \varphi_{pf0} \exp(\alpha_R t)$$

$$\alpha_R \cong - \beta / \Lambda_{pf}$$

MCNP5 1.60 includes a new capability (kopts) to calculate adjoint-weighted values for β and Λ_{pf} and therefore for Rossi α as well

Historically, Rossi α has been measured principally at LANL, ANL West, and the Japan Atomic Energy Agency

Measured values reported herein are for the delayed critical condition

Rossi α Validation Suite

Name	Fuel	Spectrum	Geometry	Moderator	Reflector
Godiva	HEU	Fast	Spherical	None	None
Flattop-25	HEU	Fast	Spherical	None	Normal Uranium
Zeus-5	HEU	Fast	Cylindrical	None	Copper
Zeus-6	HEU	Fast	Cylindrical	Steel	Copper
Zeus-1	HEU	Intermediate	Cylindrical	Graphite	Copper
Big Ten	IEU	Fast	Cylindrical	None	Depleted Uranium
STACY-30	IEU	Thermal	Cylindrical	Water	None
STACY-46	IEU	Thermal	Cylindrical	Water	Water
Jezebel-233	^{233}U	Fast	Spherical	None	None
Flattop-23	^{233}U	Fast	Spherical	None	Normal Uranium
Jezebel	Pu	Fast	Spherical	None	None
Flattop-Pu	Pu	Fast	Spherical	None	Normal Uranium
Thor	Pu	Fast	Mixed	None	Thorium

Rossi α Results for HEU and IEU Cases

Fuel	Spec-trum	Moder-ator	Reflector	Rossi α (10^4 generations/second)		
				Measured	E-VII.1β4	E-VII.0
HEU	Fast	None	None	-111 ± 2	-113 ± 2	-113 ± 1
HEU	Fast	None	Normal U	-38.2 ± 0.2	-39.8 ± 0.1	-39.7 ± 0.2
HEU	Fast	None	Copper	-79.6 ± 0.8	**-108.3 ± 0.3**	**-107.6 ± 0.8**
HEU	Fast	Steel	Copper	-37.3 ± 0.5	-41.7 ± 0.3	-41.4 ± 0.3
HEU	Intermed	Graphite	Copper	-3.38 ± 0.08	-3.60 ± 0.02	-3.63 ± 0.02
IEU	Fast	None	Depl U	-11.7 ± 0.1	-11.7 ± 0.1	-11.8 ± 0.1
IEU	Thermal	Water	None	-0.127 ± 0.003	-0.124 ± 0.003	-0.133 ± 0.003
IEU	Thermal	Water	Water	-0.106 ± 0.004	-0.108 ± 0.003	-0.104 ± 0.002

Input specifications are taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*

Agreement is reasonable except for the unmoderated Zeus case

Rossi α Results for ^{233}U and Plutonium Cases

Fuel	Spectrum	Reflector	Rossi α (10^4 generations/second)		
			Measured	ENDF/B-VII.1β4	ENDF/B-VII.0
^{233}U	Fast	None	-100 ± 1	-105 ± 1	-108 ± 1
^{233}U	Fast	Normal U	-26.7 ± 0.5	-29.3 ± 0.4	-30.2 ± 0.4
Pu	Fast	None	-64 ± 1	-64 ± 1	-65 ± 1
Pu	Fast	Normal U	-0.21.4 ± 0.5	-20.9 ± 0.3	-21.0 ± 0.3
Pu	Fast	Thorium	-19 ± 1	-21 ± 1	-20 ± 1

Input specifications are taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*

ENDF/B-VII.1β4 produces slightly improved results for ^{233}U cases but statistically insignificant changes for plutonium cases

Summary and Conclusions

For most criticality benchmarks, ENDF/B-VII.1β4 produces results that are in very close agreement with results from ENDF/B-VII.0

ENDF/B-VII.1β4 produces significantly improved results for most cases with tungsten, beryllium, cadmium, or zirconium

However, further improvement is needed for cases with beryllium

Unfortunately, a number of previously identified problems still remain, including

- Unresolved resonance range for ^{235}U
- Thermal range for ^{239}Pu
- Fast range for ^{232}Th
- Fast range for ^{237}Np
- Fast range for copper

Summary and Conclusions
(Continued)

ENDF/B-VII.1β4 and ENDF/B-VII.0 produce similar results for Rossi α that, except for the unmoderated Zeus case, are in reasonable agreement with measured values

Overall, ENDF/B-VII.1β4 can be expected to produce criticality results that are as good as those from ENDF/B-VII.0 and to produce better results for most cases with tungsten, cadmium, zirconium, or beryllium