

Lawrence Livermore National Laboratory

^{233}U Benchmarks with a Comparison to COG and MCNP Results Using ENDF/B-VII.0



Presentation to the CSEWG Data Validation Committee
at Brookhaven National Laboratory on November 3, 2009

Dave Heinrichs
Nuclear Criticality Safety Division

Lawrence Livermore National Laboratory, P.O. Box 808, L-198, Livermore, CA 94551-0808

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

Introduction

Chadwick (et al.) and **van der Marck** reported MCNP results using ENDF/B-VII.0 (**NJOY**) data for $81\text{ }^{233}\text{U}$ ICSBEP benchmarks in Nuclear Data Sheets (Dec 2006).

This paper provides corresponding results of independent COG11 calculations using ENDF/B-VII.0 (**PREPRO**) data.

Agreement between COG and MCNP is excellent but there are small but “statistically significant” differences observed for the solution benchmarks.

COG and MCNP results compare equally well with ICSBEP benchmarks.

^{233}U LANL Metal Benchmarks

No.	Evaluation	Benchmark	COG11 <i>Heinrichs</i>	MCNP4c3 <i>van der Marck</i>	Δ/σ	MCNP5 <i>Chadwick</i>	Δ/σ	Comment
1	U233-MET-FAST-001	1.0000(10)	1.0005(3)	0.9996(2)	+2.50	0.9996(1)	+2.85	Jezebel-23
2	U233-MET-FAST-005.1	1.0000(9)	0.9951(3)	0.9942(1)	+2.85	—	—	U233/Be
3	U233-MET-FAST-005.2	1.0000(6)	0.9936(3)	0.9925(1)	+3.67	—	—	U233/Be
4	U233-MET-FAST-006	1.0000(14)	0.9992(3)	0.9992(2)	+0.00	0.9991(1)	+0.28	Flattop-23

The two $^{233}\text{U}/\text{Be}$ results are $\frac{1}{2}$ to $\frac{3}{4}\%$ low.
Too few results to make other observations.

^{233}U Bettis Lattices

No.	Evaluation	Benchmark	COG11 <i>Heinrichs</i>	MCNP4c3 <i>van der Marck</i>	Δ/σ	MCNP5 <i>Chadwick</i>	Δ/σ	Comment
5	U233-COMP-THERM-001.1	1.0006(27)	—	1.0023(5)	—	1.0016(2)	—	SB-1
6	U233-COMP-THERM-001.2	1.0015(25)	1.0042(6)	1.0044(5)	-0.33	1.0043(2)	-0.16	SB-2
7	U233-COMP-THERM-001.3	1.0000(24)	1.0033(6)	1.0044(6)	-1.30	1.0040(2)	-1.11	SB-2.5
8	U233-COMP-THERM-001.4	1.0007(25)	1.0032(6)	1.0014(4)	+3.00	1.0024(2)	+1.26	SB-3
9	U233-COMP-THERM-001.5	1.0015(26)	—	1.0017(4)	—	1.0020(2)	—	SB-4
10	U233-COMP-THERM-001.6	1.0015(28)	—	1.0005(5)	—	0.9996(2)	—	SB-5
11	U233-COMP-THERM-001.7	0.9995(27)	1.0022(6)	1.0029(5)	-1.17	1.0033(2)	-1.74	SB-6
12	U233-COMP-THERM-001.8	1.0004(28)	1.0021(6)	0.9999(5)	+3.58	1.0011(2)	+1.58	SB-7

Range of calculational results appears tighter for COG:

COG 0.2 %

MCNP 0.4 %

Maximum COG11-MCNP5 difference is 0.1 ± 0.06 % Δk

Maximum MCNP4c3-MCNP5 difference is 0.1 ± 0.05 % Δk

Is this perfection*?

*See UCRL-TR-203892, “How Accurately can We Calculate Thermal Systems?”, Red Cullen et al.

²³³U ORNL Bare Solutions

No.	Evaluation	Benchmark	COG11 <i>Heinrichs</i>	MCNP4c3 <i>van der Marck</i>	Δ/σ	MCNP5 <i>Chadwick</i>	Δ/σ	Comment
13	U233-SOL-THERM-001.1	1.0000(31)	1.0019(3)	1.0016(3)	+1.00	1.0012(1)	+2.21	UST1 is bare
14	U233-SOL-THERM-001.2	1.0005(33)	1.0020(3)	1.0007(3)	+3.06	1.0013(1)	+2.21	
15	U233-SOL-THERM-001.3	1.0006(33)	1.0016(3)	1.0011(3)	+1.18	1.0010(1)	+1.90	
16	U233-SOL-THERM-001.4	0.9998(33)	1.0013(3)	1.0003(3)	+2.36	1.0008(1)	+1.58	
17	U233-SOL-THERM-001.5	0.9999(33)	1.0012(3)	1.0004(3)	+1.89	1.0003(1)	+2.85	
20	U233-SOL-THERM-008	1.0006(29)	1.0021(4)	—	—	1.0017(1)	+0.97	UST8 is bare
29	U233-SOL-THERM-013.1	0.9992(73)	1.0040(4)	—	—	1.0051(2)	-2.46	UST13 is bare
30	U233-SOL-THERM-013.2	0.9992(70)	1.0035(4)	—	—	1.0056(2)	-4.70	
31	U233-SOL-THERM-013.3	0.9992(69)	1.0046(4)	—	—	1.0059(2)	-2.91	
32	U233-SOL-THERM-013.4	0.9992(73)	1.0046(4)	—	—	1.0066(2)	-4.47	
33	U233-SOL-THERM-013.5	0.9992(67)	1.0059(4)	—	—	1.0074(2)	-3.35	
34	U233-SOL-THERM-013.6	0.9992(50)	1.0049(4)	—	—	1.0062(2)	-2.91	
35	U233-SOL-THERM-013.7	0.9992(54)	1.0046(4)	—	—	1.0066(2)	-4.47	
36	U233-SOL-THERM-013.13	0.9992(62)	1.0026(4)	—	—	1.0038(2)	-2.68	
37	U233-SOL-THERM-013.14	0.9992(51)	1.0051(4)	—	—	1.0070(2)	-4.25	
38	U233-SOL-THERM-013.15	0.9996(77)	1.0198(4)	—	—	1.0211(2)	-2.91	
39	U233-SOL-THERM-013.16	0.9996(69)	0.9931(4)	—	—	0.9937(2)	-1.34	
40	U233-SOL-THERM-013.17	0.9996(52)	0.9955(4)	—	—	0.9969(2)	-3.13	
41	U233-SOL-THERM-013.18	0.9996(20)	1.0000(4)	—	—	1.0002(2)	-0.45	
42	U233-SOL-THERM-013.19	0.9996(89)	0.9956(4)	—	—	0.9965(2)	-2.01	
43	U233-SOL-THERM-013.20	0.9996(56)	0.9986(4)	—	—	0.9999(2)	-2.91	
44	U233-SOL-THERM-013.21	0.9996(34)	1.0014(4)	—	—	1.0029(2)	-3.35	
69	U233-SOL-THERM-016.1	0.9987(37)	1.0026(4)	—	—	1.0037(2)	-2.46	UST16 is bare
71	U233-SOL-THERM-016.12	0.9992(47)	1.0037(4)	—	—	1.0047(2)	-2.24	
72	U233-SOL-THERM-016.19	1.0000(35)	0.9939(4)	—	—	0.9955(2)	-3.58	
73	U233-SOL-THERM-016.22	1.0000(34)	1.0079(4)	—	—	1.0096(2)	-3.80	
74	U233-SOL-THERM-016.25	0.9981(40)	0.9992(4)	—	—	1.0004(2)	-2.68	

-4.70 $\leq \Delta/\sigma \leq 2.85$ (range = 7.6). $\Delta k = 0.2$ % (max). Bias?

^{233}U Solutions, $\text{H}_2\text{O}/\text{CH}_2$ Reflected

No.	Evaluation	Benchmark	COG11 <i>Heinrichs</i>	MCNP4c3 <i>van der Marck</i>	Δ/σ	MCNP5 <i>Chadwick</i>	Δ/σ	Comment
18	U233-SOL-THERM-005.1	1.0000(40)	1.0010(3)	—	—	1.0019(2)	-2.50	UST5 is water reflected
19	U233-SOL-THERM-005.2	1.0000(49)	1.0045(3)	—	—	1.0051(2)	-1.66	(ORNL)
21	U233-SOL-THERM-012.1	1.0000(28)	0.9990(3)	—	—	1.0009(2)	-5.27	UST12 is water reflected
22	U233-SOL-THERM-012.2	1.0000(25)	0.9988(3)	—	—	1.0003(2)	-4.16	(ORNL)
23	U233-SOL-THERM-012.3	1.0000(23)	1.0079(3)	—	—	1.0099(2)	-5.55	
24	U233-SOL-THERM-012.4	1.0000(15)	1.0013(3)	—	—	1.0029(2)	-4.44	
25	U233-SOL-THERM-012.5	1.0000(71)	1.0034(3)	—	—	1.0052(2)	-4.99	
26	U233-SOL-THERM-012.6	1.0000(10)	1.0048(3)	—	—	1.0058(2)	-2.77	
27	U233-SOL-THERM-012.7	1.0000(38)	1.0015(3)	—	—	1.0021(2)	-1.66	
28	U233-SOL-THERM-012.8	1.0000(48)	0.9987(3)	—	—	0.9993(2)	-1.66	
65	U233-SOL-THERM-015.7	1.0000(70)	0.9865(3)	—	—	0.9882(2)	-4.71	Polyethylene reflected
66	U233-SOL-THERM-015.10	1.0000(51)	0.9883(3)	—	—	0.9902(2)	-5.27	(LLNL)
67	U233-SOL-THERM-015.17	1.0000(29)	0.9959(3)	—	—	0.9981(2)	-6.10	
68	U233-SOL-THERM-015.25	1.0000(23)	0.9970(3)	—	—	0.9989(2)	-5.27	
75	U233-SOL-THERM-017.1	0.9997(32)	1.0033(3)	—	—	1.0034(2)	-0.28	UST17 is water reflected
76	U233-SOL-THERM-017.2	1.0000(25)	0.9996(3)	—	—	1.0023(2)	-7.49	(ORNL)
77	U233-SOL-THERM-017.3	1.0001(35)	1.0039(3)	—	—	1.0045(2)	-1.66	
78	U233-SOL-THERM-017.4	0.9994(40)	1.0045(3)	—	—	1.0045(2)	+0.00	
79	U233-SOL-THERM-017.5	1.0000(29)	1.0017(3)	—	—	1.0018(2)	-0.28	
80	U233-SOL-THERM-017.6	1.0000(29)	1.0007(3)	—	—	1.0007(2)	+0.00	
81	U233-SOL-THERM-017.7	1.0000(37)	0.9997(3)	—	—	1.0002(2)	-1.39	

Negative differences indicates a bias

$\Delta/\sigma \sim 7.5$ (max) or ~ 0.3 % Δk (max) similar to bare sol'ns

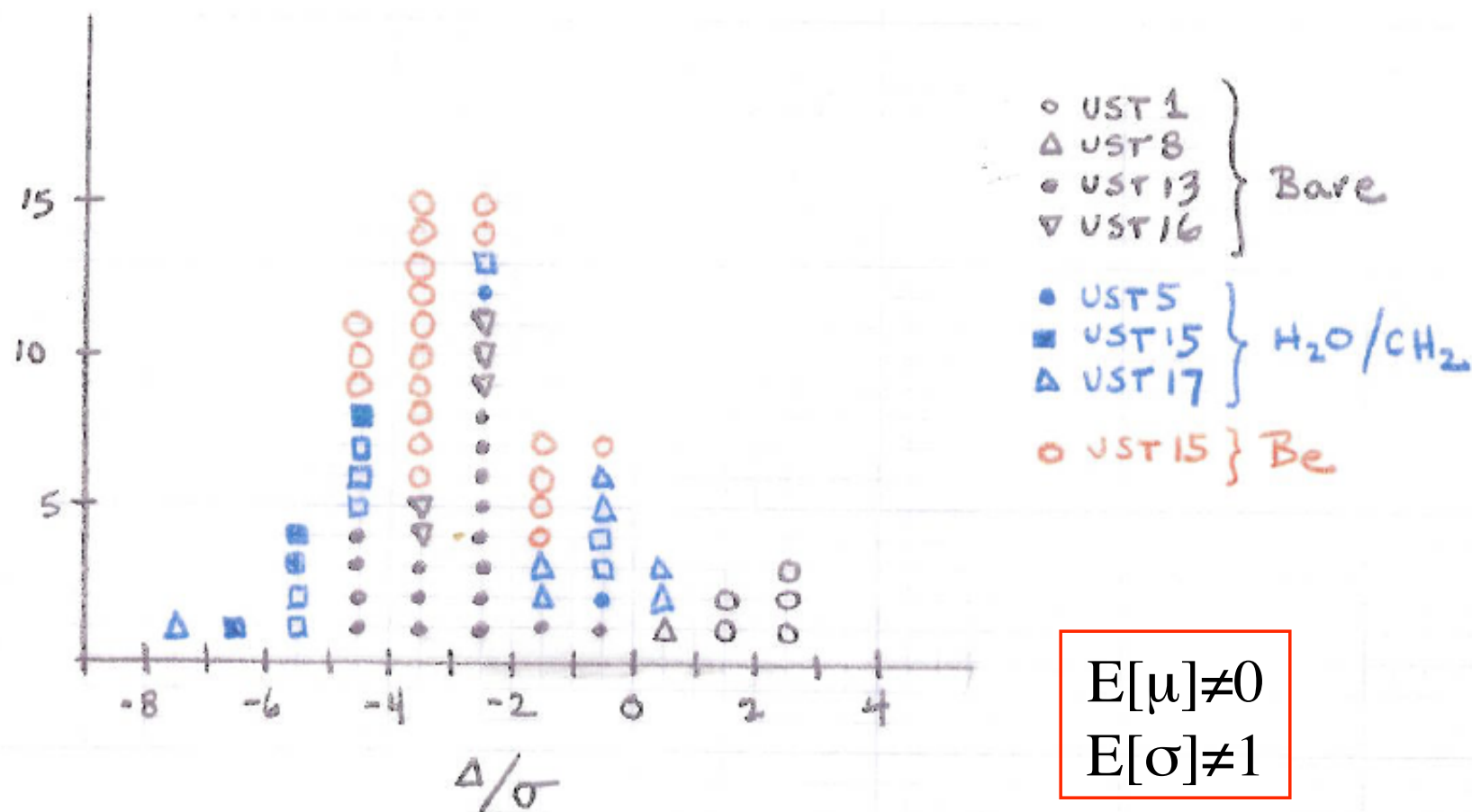
^{233}U Solutions, Be Reflected

No.	Evaluation	Benchmark	COG11 <i>Heinrichs</i>	MCNP4c3 <i>van der Marck</i>	Δ/σ	MCNP5 <i>Chadwick</i>	Δ/σ	Comments
45	U233-SOL-THERM-015.1	1.0000(75)	0.9895(3)	—	—	0.9899(2)	-1.11	UST15 is Be reflected, unless otherwise noted (LLNL)
46	U233-SOL-THERM-015.2	1.0000(70)	0.9846(3)	—	—	0.9849(2)	-0.83	
47	U233-SOL-THERM-015.3	1.0000(68)	0.9851(3)	—	—	0.9865(2)	-3.88	
48	U233-SOL-THERM-015.5	1.0000(55)	0.9851(3)	—	—	0.9863(2)	-3.33	
49	U233-SOL-THERM-015.6	1.0000(99)	0.9763(3)	—	—	0.9774(2)	-3.05	
50	U233-SOL-THERM-015.11	1.0000(75)	0.9920(3)	—	—	0.9929(2)	-2.50	
51	U233-SOL-THERM-015.12	1.0000(69)	0.9931(3)	—	—	0.9942(2)	-3.05	
52	U233-SOL-THERM-015.13	1.0000(69)	0.9909(3)	—	—	0.9921(2)	-3.33	
53	U233-SOL-THERM-015.15	1.0000(60)	0.9883(3)	—	—	0.9899(2)	-4.44	
54	U233-SOL-THERM-015.20	1.0000(79)	0.9944(3)	—	—	0.9949(2)	-1.39	
55	U233-SOL-THERM-015.21	1.0000(70)	0.9968(3)	—	—	0.9977(2)	-2.50	
56	U233-SOL-THERM-015.22	1.0000(62)	0.9949(2)	—	—	0.9961(2)	-4.24	
57	U233-SOL-THERM-015.23	1.0000(55)	0.9931(3)	—	—	0.9944(2)	-3.61	
58	U233-SOL-THERM-015.24	1.0000(51)	0.9899(3)	—	—	0.9911(2)	-3.33	
59	U233-SOL-THERM-015.26	1.0000(66)	0.9939(3)	—	—	0.9943(2)	-1.11	
60	U233-SOL-THERM-015.27	1.0000(63)	0.9976(3)	—	—	0.9988(2)	-3.33	
61	U233-SOL-THERM-015.28	1.0000(58)	0.9960(3)	—	—	0.9971(2)	-3.05	
62	U233-SOL-THERM-015.29	1.0000(51)	0.9947(3)	—	—	0.9958(2)	-3.05	
63	U233-SOL-THERM-015.30	1.0000(48)	0.9943(3)	—	—	0.9948(2)	-1.39	
64	U233-SOL-THERM-015.31	1.0000(55)	0.9934(3)	—	—	0.9949(2)	-4.16	

Negative differences indicates a bias

$\Delta/\sigma \sim 3.6$ (max) or $\sim 0.2\%$ Δk (max) similar to other sol'ns

Bias?



This mean difference is small: $\bar{\Delta} = -0.0010 \pm 0.0008 \% \Delta k$

Conclusions

COG11 and MCNP5 calculations are in agreement with ICSBEP benchmark values except in 4 cases:

- Two UMF005 cases (with Beryllium reflection)
- Two UST012 cases (benchmark uncertainties too low?)

Therefore, one code cannot be preferred over the other based on benchmark calculations.

COG11 and MCNP5 calculations are consistent within a few tenths of a percent in Δk .

Differences of one tenth of a percent are observed between van der Marck and Chadwick (et al.).

Conclusions (continued)

These consistent COG and MCNP results are believed due to enhanced collaboration in the following areas:

- Implementation of Red Cullen's treatment of high energy fission spectra in COG and MCNP
- Implementation of MCNP URRPT methods in COG
- Implementation of continuous $S(\alpha, \beta)$ in MCNP (similar to COG)

and these results provide independent verification and validation that ENDF/B-VII.0 data (for ^{233}U) has been processed and implemented correctly in COG and MCNP.

Acknowledgments

Special thanks to:

Red Cullen

Ed Lent

Rich Buck

for processing the ENDF/B-VII.0 data and implementing this data in COG11.