LA-UR-19-23348
Approved for public release; distribution is unlimited.

Title: Verification of MCNP6.2 with ENDF/B-VIII.0 Nuclear Data for Nuclear Criticality Safety Applications

Author(s): Alwin, Jennifer Louise
Brown, Forrest B.
Rising, Michael Evan

Intended for: MCNP documentation
Report

Issued: 2019-04-15

Verification of MCNP6.2 with ENDF/B-VIII.0 Nuclear Data for Nuclear Criticality Safety Applications

Jennifer L. Alwin, Forrest B. Brown, Michael E. Rising,

Monte Carlo Methods, Codes. & Applications Group (XCP-3)
Los Alamos National Laboratory, PO Box 1663, MS A143, Los Alamos NM 87545

1.0 Introduction

MCNP6.2 [1,2] was released in 2018 and is the latest production release of MCNP® available from RSICC. MCNP6.2 includes all of the standard features for nuclear criticality safety (NCS) calculations that have been available for the past 15 years, along with new features for sensitivity-uncertainty based methods using Whisper [3] for NCS validation. MCNP6.2 verification using ENDF/B-VII.1 nuclear data was previously reported in [4,5,6]. This report focuses on the initial testing and verification of MCNP6.2 using the ENDF/B-VIII.0 nuclear data that were released in 2018 [7,8,9].

The sections that follow provide:

- Guidance for NCS users on modifying existing MCNP input files to use the new ENDF/B-VIII.0 ACE nuclear data,
- Discussion of results for several ICSBEP-based benchmark suites using MCNP6.2 with ENDF/B-VII.1 and ENDF/B-VIII.0 nuclear data.

In addition, appendices provide detailed instructions for obtaining and installing the new data, a listing of the available temperatures and ZA numbers for neutron cross-sections, and a listing of the available thermal scattering S(alpha,beta) data:

Appendix A. Obtaining and installing the new ENDF/B-VIII.0 ACE nuclear data
Appendix B. ENDF/B-VIII.0-based ACE files for neutron cross-sections
Appendix C. ENDF/B-VIII.0-based ACE files for thermal scattering data, S(alpha,beta)

The detailed results from running the 3 benchmark suites with both ENDF/B-VII.1 and ENDF/B-VIII.0 nuclear data are provided in addditonal appendices:

Appendix D. Detailed results for the VALIDATION_CRITICALITY benchmark suite
Appendix E. Detailed results for the VALIDATION_CRIT_EXTENDED benchmark suite
Appendix F. Detailed results for the Whisper benchmark suite

2.0 Guidance for NCS users on modifying existing MCNP input files

After obtaining and installing the new ACE files as described in Appendix A, existing MCNP input files must usually be modified to use the new ENDF/B-VIII.0-based ACE data. Guidance for NCS practitioners is provided below.

A. Neutron cross-section ZAIDs

If the Appendix A instructions were followed to make the ENDF/B-VIII.0 ACE files the default data, then ZA numbers can be used on material and FM cards without supplying suffixes.

If instead the ENDF/B-VII.1 ACE files were chosen as the default, then explicit suffixes (e.g., .00c) must be supplied to use the ENDF/B-VIII.0 ACE data for materials and FM cards.

If suffixes are needed, refer to the information in Appendix B to select the proper suffixes. In general, for room temperature problems, all ENDF/B-VII.1 suffixes of .80c should be changed to .00c on all material cards and FM cards.

B. Thermal scattering data

Because the new ENDF/B-VIII.0 ACE data for thermal scattering has significant changes in the ACE file names, all MT cards need to be reviewed and appropriately modified. Appendix C lists the new names to be used on the MT cards. Typical changes might be:

lwtr	→	h-h2o
hwtr	→	d-d2o, o-d2o
poly	→	h-poly
be-o	→	be-beo
o-be	→	o-beo
be	→	be-met
h-zr	→	h-zrh
zr-h	→	zr-zrh
grph	→	grph or grph10 or grph30

For room temperature data (if it exists), the suffix to use is .80t. (There is no room temperature data for h-ice, o-ice, lmeth, orthoD, orthoH, paraD, paraH, or smeth.)

There are new ACE data files for H and O in ice, H in lucite, and Si and C in silicon carbide. The carbon data (grph) are also now available for graphite at 10% porosity, 30% porosity, or solid.

C. Special treatment for Carbon

The previous ENDF/B-VII.1 ACE data included data for natural, elemental carbon only, with ZA = 6000. The new ENDF/B-VIII.0 ACE data does <u>not</u> include data for elemental carbon – the specific carbon isotopes 6012 and 6013 must be used.

Material and FM cards that previously used 6000 or 6000.80c must be changed to use 6012 or 6012.00c or a mixture of 6012.00c (98.93 atom %) plus 6013.00c (1.07 atom %). These changes should be made to both material and FM cards.

3.0 Comparison of results for several ICSBEP-based benchmark suites using MCNP6.2 with ENDF/B-VII.1 and ENDF/B-VIII.0 nuclear data.

Three suites of verification-validation criticality benchmark problems were run in late-2018 and early-2019 to verify that MCNP6.2 performs correctly for NCS applications using either ENDF/B-VII.1- or ENDF/B-VIII.0-based ACE files:

- **VALIDATION_CRITICALITY** [10] – 31 ICSBEP problems,
- **VALIDATION_CRIT_EXTENDED** [11] - 119 ICSBEP problems,
- **Whisper Benchmark Suite** [12] – 1101 ICSBEP problems.

Detailed results from the comparisons are shown in Appendices D, E, and F.

The criticality verification-validation suites were run on MacOS, Linux, or Windows systems with MCNP6.2 (the 2018 release) or MCNP6.2.1 (the 2019 version, with a few minor changes that do not affect criticality calculations). For MacOS, the suites were run on a Mac Pro computer using 64-bit executables, 12-core Xeon processor, MacOS 10.12.6, and 12 MCNP threads. For Linux, the suites were run on a single node of a LANL cluster, with 64-bit executables, 2-cpus with 18-core Xeon processors, RedHat 7 Linux, and 18 MCNP threads. For Windows, the suites were run on a Windows laptop using 64-bit executable, a quad-core I7-4930MX with hyperthreading, Windows 10, and 4 MCNP threads.

A. VALIDATION_CRITICALITY Suite

Detailed results for this benchmark suite are shown in Appendix D. **Table D-1** shows the K_{eff} results for 31 ICSBEP benchmark problems using ENDF/B-VII.1 and ENDF/B-VIII.0 nuclear data**. Table D-2** shows the differences in results relative to the benchmark experiments. In reviewing the results in the 2 tables, the ENDF/B-VIII.0 results are generally slightly closer to experiment, but the differences from ENDF/B-VII.1 are not large. No specific results stand out as unusual or suspicious.

B. VALIDATION_CRIT_EXTENDED Suite

Detailed results for this benchmark suite are shown in Appendix E. This benchmark suite includes 119 ICSBEP benchmark problems. Results are shown in **Table E-1 and Figure E-1**. Similar to the results from VALIDATION_CRITICALITY, the results are reasonable, with some general improvement and no glaring differences or unexpected large differences.

C. Whisper Benchmark Suite

Detailed results for this benchmark suite are shown in Appendix F. **Table F-1** provides a summary of the overall differences, broken down into overall, Pu, HEU, MIX, IEU, LEU, and U-233 benchmarks. **Figure F-1** shows the overall distribution of differences, and **Figure F-2** shows the overall comparison of results. Tables F-2 through F-5 and Figures F-3 through F-6 show detailed comparisons for the separate groups of Pu, HEU, MIX, IEU, LEU, and U-233 benchmarks. Again some improvements are observed, with no significant or unexpected differences in results.

4.0 SUMMARY AND CONCLUSIONS

The general conclusions from this testing are:

- MCNP6.2 performs correctly using either ENDF/B-VII.1 or ENDF/B-VIII.0 nuclear data for NCS applications. No errors or unexpected code calculation behavior were observed.
- No significant large differences are apparent between ENDF/B-VII.1 and ENDF/B-VIII.0 results. In general, most results are comparable or slightly closer to experiment with ENDF/B-VIII.0, and some results are slightly worse.
- The LANL Monte Carlo group recommends that NCS practitioners upgrade to using the ENDF/B-VIII.0 nuclear data. Of course, much effort for code and data validation is required to make such an upgrade, and each DOE NCS site will have to assess when it is practical to make the transition. We have found no glaring changes that would prohibit an upgrade to ENDF/B-VIII.0 nuclear data. The advantages to using the most current and best nuclear data are obvious.

ACKNOWLEDGMENTS

This work was supported by the US DOE-NNSA Nuclear Criticality Safety Program.

REFERENCES

1. C.J. Werner, J.S. Bull, et al., “MCNP6.2 Release Notes”, LA-UR-18-20808 (2018).
2. C.J. Werner (editor), “MCNP Users Manual – Code Version 6.2”, LA-UR-17-29981 (2017).
3. B.C. Kiedrowski, F.B. Brown, et al., “Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Upper Subcritical Limits”, *Nucl. Sci. Eng.* **181**, 17-47 [also LA-UR-14-26558] (2015).
4. F.B. Brown, M.E. Rising, J.L. Alwin, “Verification of MCNP6.2 for Nuclear Criticality Safety Applications”, LA- UR-18-25535 (2018).
5. F.B. Brown, M.E. Rising, “Verification of MCNP6.2 Release for Nuclear Criticality Safety Applications”, LA- UR-17-23822 (2017).
6. F.B. Brown, M.E. Rising, “Verification of MCNP6.1, MCNP6.1.1, and MCNP6.2-pre for Criticality Safety Applications”, LA-UR-16-24308 (2016).
7. J.L. Conlin, W. Haeck, et al., “Release of ENDF/B-VIII.0-Based ACE Data Files”, LA-UR-18-24034 (2018).
8. J.L. Conlin, et al., web pages at nucleardata.lanl.gov
9. D.K. Parsons, “NJOY Processing of ENDF/B-VIII.0 Thermal Scattering Files”, LA-UR-18-25096 (2018).
10. Russell D. Mosteller, "Validation Suites for MCNP," Proceedings of the American Nuclear Society Radiation Protection and Shielding Division 12th Biennial Topical Meeting, Santa Fe, New Mexico (April 2002). (LA-UR-02-0878)
11. R.D. Mosteller "An Expanded Criticality Validation Suite for MCNP", LA-UR-10-06230 Rev3 (2010).
12. B.C. Kiedrowski, et al., "Validation of MCNP6.1 for Criticality Safety of Pu-Metal, -Solution, and -Oxide Systems", LA-UR-14-23352 (2014)

Appendix A. Obtaining and installing the new ENDF/B-VIII.0 ACE nuclear data

The new ACE files based on ENDF/B-VIII.0 nuclear data are available from the website **nucleardata.lanl.gov**. While that website has instructions for installing the data on your computer, it is suggested that NCS users instead follow the directions below.

(1) On your computer, create a temporary folder (directory) for downloading and decompressing the data files. Make sure that about 50 GB of disk space is available to handle the new data.

(2) Go to the website nucleardata.lanl.gov, and then download these files into your temporary folder:

Windows: Lib80X.zip (approx.. 7 GB), ENDF80SaB.zip (approx.. 2.5 GB)

Linux/Mac: Lib80X.tgz (approx. 7 GB), ENDF80SaB.tgz (approx.. 2.5 GB)

(3) Decompress the downloaded files:

```
Windows:    unzip  Lib80X.zip
            unzip  ENDF80SaB.zip

Linux/Mac:  tar  xfz  Lib80X.tgz
            tar  xfz  ENDF80SaB.tgz
```

The expanded data files require about 45 GB of disk storage space.

(4) Move the new data folders into your existing MCNP data storage folder:

```
Windows:    move  Lib80X       %DATAPATH%\xdata
            move  ENDF80SaB    %DATAPATH%\xdata

Linux/Mac:  mv  Lib80X        $DATAPATH/xdata
            mv  ENDF80SaB     $DATAPATH/xdata
```

Note that the instructions in this step differ from the instructions on the nucleardata website. The new data are moved into *xdata* folder, rather than the higher-level main data folder.

(5) Download these files from the mcnp.lanl.gov website:

xsdir_mcnp6.2_endf71
xsdir_mcnp6.2_endf80

(6) Move the 2 files into the existing MCNP data storage folder:

```
Windows:    move  xsdir_mcnp6.2_endf71    %DATAPATH%
            move  xsdir_mcnp6.2_endf80    %DATAPATH%

Linux/Mac:  mv  xsdir_mcnp6.2_endf71    $DATAPATH
            mv  xsdir_mcnp6.2_endf80    $DATAPATH
```

(7) Rename the existing xsdir_mcnp6.2:

Windows:
```
cd  %DATAPATH%
rename   xsdir_mcnp6.2    xsdir_mcnp6.2_old
```

Linux/Mac:
```
cd  $DATAPATH
mv  xsdir_mcnp6.2    xsdir_mcnp6.2_old
```

(8) Decide what the default data should be and recreate the xsdir_mcnp6.2 file:

Both xsdir files (xsdir_mcnp6.2_endf71 and xsdir_mcnp6.2_endf80) contain entries that include the ENDF/B-VII.1 and ENDF/B-VIII.0 data, but provide different defaults. The first file defaults ZAIDs without suffixes to the ENDDF/B-VII.1 ACE data; the second file defaults ZAIDs without suffixes to the ENDF/B-VIII.0 ACE data.

It is up to the NCS user (or their site) to decide whether the default data for ZAIDs without suffixes should be the ENDF/B-VII.1 or ENDF/B-VIII.0 ACE files.

To make the default data be ENDF/B-VII.1:

Windows:
```
cd %DATAPATH%
copy  xsdir_mcnp6.2_endf71  xsdir_mcnp6.2
```

Linux/Mac:
```
cd $DATAPATH
cp    xsdir_mcnp6.2_endf71  xsdir_mcnp6.2
```

To make the default data be ENDF/B-VIII.0:

Windows:
```
cd %DATAPATH%
copy  xsdir_mcnp6.2_endf80  xsdir_mcnp6.2
```

Linux/Mac:
```
cd $DATAPATH
cp    xsdir_mcnp6.2_endf80  xsdir_mcnp6.2
```

(9) Run a test problem to verify that the data files were installed and configured correctly:
For each run, examine the mcnp6.2 output file to check that the correct ACE data files were used.

Default
```
Godiva - simple case
1 1 -18.74 -1 imp:n=1
2 0         1 imp:n=0

1    so 8.741

kcode 10000 1.0 10 110
ksrc  0. 0. 0.
m1  92235    -94.73
    92238     -5.27
```

Explicit ENDF/B-VII.1
```
Godiva - simple case
1 1 -18.74 -1 imp:n=1
2 0         1 imp:n=0

1    so 8.741

kcode 10000 1.0 10 110
ksrc  0. 0. 0.
m1  92235.80c -94.73
    92238.80c  -5.27
```

Explicit ENDF/B-VIII.0
```
Godiva - simple case
1 1 -18.74 -1 imp:n=1
2 0         1 imp:n=0

1    so 8.741

kcode 10000 1.0 10 110
ksrc  0. 0. 0.
m1  92235.00c  -94.73
    92238.00c   -5.27
```

Appendix B. ENDF/B-VIII.0-based ACE files for neutron cross-sections

The release of ACE files based on ENDF/B-VIII.0 includes neutron cross-section data for 556 isotopes and thermal scattering S(alpha,beta) data for 33 materials [7,8]. No data is provided for elements; the elemental carbon data provided in ENDF/B-VII.1 is not supported in ENDF/B-VIII.0.

The ACE files for neutron cross-section data are provided at 7 temperatures. The temperatures and ZAID extensions are:

Temperature (K)	ZAID Extension
293.6	.00c
600	.01c
900	.02c
1200	.03c
2500	.04c
0.1	.05c
250	.06c

The ACE files for neutron cross-section data are available for the ZA numbers listed below, where ZA = Z*1000 + A. For metastable isotopes, ZA = Z*1000 + A + S*100, where S is the excited state number. (There is an exception to this for ^{242}Am. For historical reasons 95242 is for the first metastable state of ^{242}Am and 95642 is for ground-state ^{242}Am.)

The available ZAs are (see footnotes at end of table):

1001	1002	1003	2003	2004	3006	3007	4007	4009	5010
5011	6012*	6013*	7014	7015	8016	8017	8018*	9019	10020*
10021*	10022*	11022	11023	12024	12025	12026	13426†	13027	14028
14029	14030	14031*	14032*	15031	16032	16033	16034	16035*	16036
17035	17036*	17037	18036	18037*	18038	18039*	18040	18041*	19039
19040	19041	20040	20041*	20042	20043	20044	20045*	20046	20047*
20048	21045	22046	22047	22048	22049	22050	23049*	23050	23051
24050	24051*	24052	24053	24054	25054*	25055			
26054	26055*	26056	26057	26058	27058	27458†	27059	28058	28059
28060	28061	28062	28063*	28064	29063	29064*	29065	30064	30065
30066	30067	30068	30069*	30070	31069	31070*	31071	32070	32071*
32072	32073	32074	32075*	32076	33073*	33074	33075	34074	34075*
34076	34077	34078	34079	34080	34081*	34082	35079	35080*	35081
36078	36079*	36080	36081*	36082	36083	36084	36085	36086	37085

37086	37087	38084	38085*	38086	38087	38088	38089	38090	39089
39090	39091	40090	40091	40092	40093	40094	40095	40096	41093
41094	41095	42092	42093*	42094	42095	42096	42097	42098	42099
42100	43098*	43099	44096	44097*	44098	44099	44100	44101	44102
44103	44104	44105	44106	45103	45104*	45105	46102	46103*	46104
46105	46106	46107	46108	46109*	46110	47107	47108*	47109	47510†
47111	47112*	47113*	47114*	47115*	47116*	47117*	47518†	48106	48107*
48108	48109*	48110	48111	48112	48113	48114	48515†	48116	49113
49114*	49115	50112	50113	50114	50115	50116	50117	50118	50119
50120	50521†	50122	50123	50124	50125	50126	51121	51122*	51123
51124	51125	51126	52120	52121*	52521†	52122	52123	52124	52125
52126	52527†	52128	52529†	52130	52131*	52531†	52132	53127	53128*
53129	53130	53131	53132*	53532†	53133*	53134*	53135	54123	54124
54125*	54126	54127*	54128	54129	54130	54131	54132	54133	54134
54135	54136	55133	55134	55135	55136	55137	56130	56131*	56132
56133	56134	56135	56136	56137	56138	56139*	56140	57138	57139
57140	58136	58137*	58537†	58138	58139	58140	58141	58142	58143
58144	59141	59142	59143	60142	60143	60144	60145	60146	60147
60148	60149*	60150	61143*	61144*	61145*	61146*	61147	61148	61548†
61149	61150*	61151	62144	62145*	62146*	62147	62148	62149	62150
62151	62152	62153	62154	63151	63152	63153	63154	63155	63156
63157	64152	64153	64154	64155	64156	64157	64158	64159	64160
65158*	65159	65160	65161*	66154*	66155*	66156	66157*	66158	66159*
66160	66161	66162	66163	66164	67165	67566†	68162	68163*	68164
68165*	68166	68167	68168	68169*	68170	69168	69169	69170	69171*
70168*	70169*	70170*	70171*	70172*	70173*	70174*	70175*	70176*	71175
71176	72174	72175*	72176	72177	72178	72179	72180	72181*	72182*
73180	73181	73182	74180	74181*	74182	74183	74184	74185*	74186
75185	75586†	75187	76184*	76185*	76186*	76187*	76188*	76189*	76190*
76191*	76192*	77191	77192*	77193	77594†	78190*	78191*	78192*	78193*
78194*	78195*	78196*	78197*	78198*	79197	80196	80197*	80597†	80198
80199	80200	80201	80202	80203*	80204	81203	81204*	81205	82204
82205*	82206	82207	82208	83209	83610†	84208*	84209*	84210*	88223
88224	88225	88226							

89225	89226	89227	90227	90228	90229	90230	90231	90232	90233
90234	91229	91230	91231	91232	91233	92230	92231	92232	92233
92234	92235	92236	92237	92238	92239	92240	92241	93234	93235
93236	93636†	93237	93238	93239	94236	94237	94238	94239	94240
94241	94242	94243	94244	94245*	94246	95240	95241	95642†	95242

95243	95244	95644†	96240	96241	96242	96243	96244	96245	96246
96247	96248	96249	96250	97245	97246	97247	97248	97249	97250
98246	98247*	98248	98249	98250	98251	98252	98253	98254	99251
99252	99253	99254	99654†	99255	100255				

* New evaluations in ENDF/B-VIII.0.
† Excited state evaluations

Appendix C. ENDF/B-VIII.0-based ACE files for thermal scattering data, S(alpha,beta)

h-h2o	hydrogen in light water
h-ice	hydrogen in solid light water (ice)
o-ice	oxygen in solid light water (ice)
h-luci	hydrogen in Lucite
h-poly	hydrogen in polyethylene
h-yh2	hydrogen in yttrium-hydride
y-yh2	yttrium in yttrium-hydride
h-zrh	hydrogen in zirconium-hydride
zr-zrh	zirconium in zirconium-hydride
d-d2o	deuterium in heavy water
o-d2o	oxygen in heavy water
be-beo	beryllium in beryllium-oxide
o-beo	oxygen in beryllium-oxide
be-met	beryllium metal
grph10	10% porous graphite
grph30	30% porous graphite
grph	crystalline graphite
sio2	silicon-dioxide
si-sic	silicon in silicon-carbide
c-sic	carbon in silicon carbide
benz	benzene
n-un	nitrogen in uranium-nitride
u-un	uranium in uranium-nitride
o-uo2	oxygen in uranium-dioxide
u-uo2	uranium in uranium-dioxide
al-27	aluminum-27 metal
fe-56	iron-56 metal
lmeth	hydrogen in liquid methane
smeth	hydrogen in solid methane
paraD	liquid para-deuterium
paraH	liquid para-hydrogen
orthoD	liquid ortho-deuterium
orthoH	liquid ortho-hydrogen

For room temperature data (if it exists), the suffix to use is .80t. (There is no room temperature data for h-ice, o-ice, lmeth, orthoD, orthoH, paraD, paraH, or smeth.)

The set of available S(alpha,beta) ACE files are listed below, with names, ZAIDs, and temperatures.

S(a,B)	AWR	Temp(MeV)	Temp K
al-27.80t	26.74975	2.530E-08	294
al-27.81t	26.74975	1.724E-09	20
al-27.82t	26.74975	6.894E-09	80
al-27.83t	26.74975	3.447E-08	400
al-27.84t	26.74975	5.170E-08	600
al-27.85t	26.74975	6.894E-08	800
be-beo.80t	8.93478	2.530E-08	294
be-beo.81t	8.93478	3.447E-08	400
be-beo.82t	8.93478	4.309E-08	500
be-beo.83t	8.93478	5.170E-08	600
be-beo.84t	8.93478	6.032E-08	700
be-beo.85t	8.93478	6.894E-08	800
be-beo.86t	8.93478	8.617E-08	1000
be-beo.87t	8.93478	1.034E-07	1200
be-met.80t	8.93478	2.551E-08	296
be-met.81t	8.93478	3.447E-08	400
be-met.82t	8.93478	4.309E-08	500
be-met.83t	8.93478	5.170E-08	600
be-met.84t	8.93478	6.032E-08	700
be-met.85t	8.93478	6.894E-08	800
be-met.86t	8.93478	8.617E-08	1000
be-met.87t	8.93478	1.034E-07	1200
benz.80t	0.999167	2.551E-08	296
benz.81t	0.999167	3.016E-08	350
benz.82t	0.999167	3.447E-08	400
benz.83t	0.999167	3.878E-08	450
benz.84t	0.999167	4.309E-08	500
benz.85t	0.999167	5.170E-08	600
benz.86t	0.999167	6.894E-08	800
benz.87t	0.999167	8.617E-08	1000
c-sic.80t	11.89365	2.585E-08	300
c-sic.81t	11.89365	3.447E-08	400
c-sic.82t	11.89365	4.309E-08	500
c-sic.83t	11.89365	5.170E-08	600
c-sic.84t	11.89365	6.032E-08	700
c-sic.85t	11.89365	6.894E-08	800
c-sic.86t	11.89365	8.617E-08	1000
c-sic.87t	11.89365	1.034E-07	1200
d-d2o.80t	1.9968	2.530E-08	294
d-d2o.81t	1.9968	2.444E-08	284
d-d2o.82t	1.9968	2.585E-08	300
d-d2o.83t	1.9968	2.789E-08	324
d-d2o.84t	1.9968	3.016E-08	350
d-d2o.85t	1.9968	3.220E-08	374
d-d2o.86t	1.9968	3.447E-08	400
d-d2o.87t	1.9968	3.650E-08	424
d-d2o.88t	1.9968	3.878E-08	450
d-d2o.89t	1.9968	4.081E-08	474
d-d2o.90t	1.9968	4.309E-08	500
d-d2o.91t	1.9968	4.512E-08	524
d-d2o.92t	1.9968	4.740E-08	550
d-d2o.93t	1.9968	4.943E-08	574
d-d2o.94t	1.9968	5.170E-08	600
d-d2o.95t	1.9968	5.374E-08	624
d-d2o.96t	1.9968	5.601E-08	650
fe-56.80t	55.45443	2.530E-08	294
fe-56.81t	55.45443	1.724E-09	20
fe-56.82t	55.45443	6.894E-09	80
fe-56.83t	55.45443	3.447E-08	400
fe-56.84t	55.45443	5.170E-08	600
fe-56.85t	55.45443	6.894E-08	800
grph.80t	11.89365	2.551E-08	296
grph.81t	11.89365	3.447E-08	400
grph.82t	11.89365	4.309E-08	500
grph.83t	11.89365	5.170E-08	600
grph.84t	11.89365	6.032E-08	700
grph.85t	11.89365	6.894E-08	800
grph.86t	11.89365	8.617E-08	1000
grph.87t	11.89365	1.034E-07	1200
grph.88t	11.89365	1.379E-07	1600
grph10.80t	11.89365	2.551E-08	296
grph10.81t	11.89365	3.447E-08	400
grph10.82t	11.89365	4.309E-08	500
grph10.83t	11.89365	5.170E-08	600
grph10.84t	11.89365	6.032E-08	700
grph10.85t	11.89365	6.894E-08	800
grph10.86t	11.89365	8.617E-08	1000
grph10.87t	11.89365	1.034E-07	1200
grph10.88t	11.89365	1.379E-07	1600
grph30.80t	11.89365	2.551E-08	296

grph30.81t	11.89365	3.447E-08	400
grph30.82t	11.89365	4.309E-08	500
grph30.83t	11.89365	5.170E-08	600
grph30.84t	11.89365	6.032E-08	700
grph30.85t	11.89365	6.894E-08	800
grph30.86t	11.89365	8.617E-08	1000
grph30.87t	11.89365	1.034E-07	1200
grph30.88t	11.89365	1.379E-07	1600
h-h2o.80t	0.999167	2.530E-08	294
h-h2o.81t	0.999167	2.444E-08	284
h-h2o.82t	0.999167	2.585E-08	300
h-h2o.83t	0.999167	2.789E-08	324
h-h2o.84t	0.999167	3.016E-08	350
h-h2o.85t	0.999167	3.220E-08	374
h-h2o.86t	0.999167	3.447E-08	400
h-h2o.87t	0.999167	3.650E-08	424
h-h2o.88t	0.999167	3.878E-08	450
h-h2o.89t	0.999167	4.081E-08	474
h-h2o.90t	0.999167	4.309E-08	500
h-h2o.91t	0.999167	4.512E-08	524
h-h2o.92t	0.999167	4.740E-08	550
h-h2o.93t	0.999167	4.943E-08	574
h-h2o.94t	0.999167	5.170E-08	600
h-h2o.95t	0.999167	5.374E-08	624
h-h2o.96t	0.999167	5.601E-08	650
h-h2o.97t	0.999167	6.894E-08	800
h-ice.80t	0.999167	9.910E-09	115
h-ice.81t	0.999167	1.621E-08	188
h-ice.82t	0.999167	1.794E-08	208
h-ice.83t	0.999167	1.966E-08	228
h-ice.84t	0.999167	2.009E-08	233
h-ice.85t	0.999167	2.138E-08	248
h-ice.86t	0.999167	2.182E-08	253
h-ice.87t	0.999167	2.311E-08	268
h-ice.88t	0.999167	2.354E-08	273
h-luci.80t	0.999167	2.585E-08	300
h-poly.80t	0.999167	2.530E-08	294
h-poly.81t	0.999167	6.635E-09	77
h-poly.82t	0.999167	1.689E-08	196
h-poly.83t	0.999167	2.008E-08	233
h-poly.84t	0.999167	2.585E-08	300
h-poly.85t	0.999167	2.611E-08	303
h-poly.86t	0.999167	2.697E-08	313
h-poly.87t	0.999167	2.783E-08	323
h-poly.88t	0.999167	2.870E-08	333
h-poly.89t	0.999167	2.783E-08	323
h-poly.90t	0.999167	2.870E-08	333
h-yh2.80t	0.999167	2.530E-08	294
h-yh2.81t	0.999167	3.447E-08	400
h-yh2.82t	0.999167	4.309E-08	500
h-yh2.83t	0.999167	5.170E-08	600
h-yh2.84t	0.999167	6.032E-08	700
h-yh2.85t	0.999167	6.894E-08	800
h-yh2.86t	0.999167	8.617E-08	1000
h-yh2.87t	0.999167	1.034E-07	1200
h-yh2.88t	0.999167	1.206E-07	1400
h-zrh.80t	0.999167	2.551E-08	296
h-zrh.81t	0.999167	3.447E-08	400
h-zrh.82t	0.999167	4.309E-08	500
h-zrh.83t	0.999167	5.170E-08	600
h-zrh.84t	0.999167	6.032E-08	700
h-zrh.85t	0.999167	6.894E-08	800
h-zrh.86t	0.999167	8.617E-08	1000
h-zrh.87t	0.999167	1.034E-07	1200
lmeth.80t	0.999167	8.617E-09	100
n-un.80t	13.88278	2.551E-08	296
n-un.81t	13.88278	3.447E-08	400
n-un.82t	13.88278	4.309E-08	500
n-un.83t	13.88278	5.170E-08	600
n-un.84t	13.88278	6.032E-08	700
n-un.85t	13.88278	6.894E-08	800
n-un.86t	13.88278	8.617E-08	1000
n-un.87t	13.88278	1.034E-07	1200
o-beo.80t	15.85751	2.530E-08	294
o-beo.81t	15.85751	3.447E-08	400
o-beo.82t	15.85751	4.309E-08	500
o-beo.83t	15.85751	5.170E-08	600
o-beo.84t	15.85751	6.032E-08	700
o-beo.85t	15.85751	6.894E-08	800
o-beo.86t	15.85751	8.617E-08	1000
o-beo.87t	15.85751	1.034E-07	1200
o-d2o.80t	15.85751	2.530E-08	294
o-d2o.81t	15.85751	2.444E-08	284
o-d2o.82t	15.85751	2.585E-08	300
o-d2o.83t	15.85751	2.789E-08	324
o-d2o.84t	15.85751	3.016E-08	350

o-d2o.85t	15.85751	3.220E-08	374
o-d2o.86t	15.85751	3.447E-08	400
o-d2o.87t	15.85751	3.650E-08	424
o-d2o.88t	15.85751	3.878E-08	450
o-d2o.89t	15.85751	4.081E-08	474
o-d2o.90t	15.85751	4.309E-08	500
o-d2o.91t	15.85751	4.512E-08	524
o-d2o.92t	15.85751	4.740E-08	550
o-d2o.93t	15.85751	4.943E-08	574
o-d2o.94t	15.85751	5.170E-08	600
o-d2o.95t	15.85751	5.374E-08	624
o-d2o.96t	15.85751	5.601E-08	650
o-ice.80t	15.85751	9.910E-09	115
o-ice.81t	15.85751	1.621E-08	188
o-ice.82t	15.85751	1.794E-08	208
o-ice.83t	15.85751	1.966E-08	228
o-ice.84t	15.85751	2.009E-08	233
o-ice.85t	15.85751	2.138E-08	248
o-ice.86t	15.85751	2.182E-08	253
o-ice.87t	15.85751	2.311E-08	268
o-ice.88t	15.85751	2.354E-08	273
o-uo2.80t	15.85751	2.551E-08	296
o-uo2.81t	15.85751	3.447E-08	400
o-uo2.82t	15.85751	4.309E-08	500
o-uo2.83t	15.85751	5.170E-08	600
o-uo2.84t	15.85751	6.032E-08	700
o-uo2.85t	15.85751	6.894E-08	800
o-uo2.86t	15.85751	8.617E-08	1000
o-uo2.87t	15.85751	1.034E-07	1200
orthoD.80t	1.9968	1.637E-09	19
orthoH.80t	0.999167	1.724E-09	20
paraD.80t	1.9968	1.637E-09	19
paraH.80t	0.999167	1.724E-09	20
si-sic.80t	27.737	2.585E-08	300
si-sic.81t	27.737	3.447E-08	400
si-sic.82t	27.737	4.309E-08	500
si-sic.83t	27.737	5.170E-08	600
si-sic.84t	27.737	6.032E-08	700
si-sic.85t	27.737	6.894E-08	800
si-sic.86t	27.737	8.617E-08	1000
si-sic.87t	27.737	1.034E-07	1200
sio2.80t	15.85751	2.530E-08	294
sio2.81t	15.85751	3.016E-08	350
sio2.82t	15.85751	3.447E-08	400
sio2.83t	15.85751	4.309E-08	500
sio2.84t	15.85751	6.894E-08	800
sio2.85t	15.85751	8.617E-08	1000
sio2.86t	15.85751	9.479E-08	1100
smeth.80t	0.999167	1.896E-09	22
u-un.80t	236.0058	2.551E-08	296
u-un.81t	236.0058	3.447E-08	400
u-un.82t	236.0058	4.309E-08	500
u-un.83t	236.0058	5.170E-08	600
u-un.84t	236.0058	6.032E-08	700
u-un.85t	236.0058	6.894E-08	800
u-un.86t	236.0058	8.617E-08	1000
u-un.87t	236.0058	1.034E-07	1200
u-uo2.80t	236.0058	2.551E-08	296
u-uo2.81t	236.0058	3.447E-08	400
u-uo2.82t	236.0058	4.309E-08	500
u-uo2.83t	236.0058	5.170E-08	600
u-uo2.84t	236.0058	6.032E-08	700
u-uo2.85t	236.0058	6.894E-08	800
u-uo2.86t	236.0058	8.617E-08	1000
u-uo2.87t	236.0058	1.034E-07	1200
y-yh2.80t	88.1421	2.530E-08	294
y-yh2.81t	88.1421	3.447E-08	400
y-yh2.82t	88.1421	4.309E-08	500
y-yh2.83t	88.1421	5.170E-08	600
y-yh2.84t	88.1421	6.032E-08	700
y-yh2.85t	88.1421	6.894E-08	800
y-yh2.86t	88.1421	8.617E-08	1000
y-yh2.87t	88.1421	1.034E-07	1200
y-yh2.88t	88.1421	1.206E-07	1400
zr-zrh.80t	89.1324	2.551E-08	296
zr-zrh.81t	89.1324	3.447E-08	400
zr-zrh.82t	89.1324	4.309E-08	500
zr-zrh.83t	89.1324	5.170E-08	600
zr-zrh.84t	89.1324	6.032E-08	700
zr-zrh.85t	89.1324	6.894E-08	800
zr-zrh.86t	89.1324	8.617E-08	1000
zr-zrh.87t	89.1324	1.034E-07	1200

Appendix D. Detailed results for VALIDATION_CRITICALITY benchmark suite

Table D-1. Results for VALIDATION_CRITICALITY Suite

Benchmark = Benchmark values from experiments
621_71_mac = mcnp6.2.1 + Intel-18 + endf/b-vii.1 + macos
621_80_mac = mcnp6.2.1 + Intel-18 + endf/b-viii.0 + macos

*'s indicate differences > 1, 2, or 3 std

	Benchmark		621_71_mac		621_80_mac	
	keff	std	keff	std	keff	std
U233 Benchmarks						
JEZ233	1.0000	(10)	1.0001	(2)	1.0004	(2)
FLAT23	1.0000	(14)	0.9986	(2)	1.0000	(2)
UMF5C2	1.0000	(30)	0.9953	(2)*	0.9974	(2)
FLSTF1	1.0000	(83)	0.9851	(5)*	0.9814	(5)**
SB25	1.0000	(23)	1.0011	(4)	1.0001	(4)
ORNL11	1.0006	(28)	1.0015	(2)	0.9996	(2)
HEU Benchmarks						
GODIVA	1.0000	(10)	1.0003	(2)	0.9999	(2)
TT2C11	1.0000	(38)	1.0006	(2)	0.9988	(2)
FLAT25	1.0000	(30)	1.0037	(2)*	1.0013	(2)
GODIVR	0.9985	(11)	0.9999	(2)*	0.9996	(4)
UH3C6	1.0000	(47)	0.9953	(4)	0.9982	(2)
ZEUS2	0.9997	(8)	0.9963	(2)***	0.9994	(4)
SB5RN3	1.0015	(28)	0.9956	(4)**	0.9935	(4)**
ORNL10	1.0015	(26)	0.9992	(1)	0.9982	(2)*
IEU Benchmarks						
IMF03	1.0000	(17)	1.0030	(2)*	0.9999	(2)
BIGTEN	0.9948	(13)	0.9945	(2)	0.9943	(2)
IMF04	1.0000	(30)	1.0076	(2)**	1.0053	(2)*
ZEBR8H	1.0300	(25)	1.0191	(2)***	1.0230	(2)**
ICT2C3	1.0017	(44)	1.0040	(2)	1.0046	(2)
STACY36	0.9988	(13)	0.9989	(2)	0.9984	(2)
LEU Benchmarks						
BAWXI2	1.0007	(11)	1.0008	(2)	1.0008	(2)
LST2C2	1.0024	(37)	0.9960	(2)*	0.9959	(2)*
Pu Benchmarks						
JEZPU	1.0000	(20)	0.9995	(2)	0.9998	(2)
JEZ240	1.0000	(20)	0.9999	(2)	1.0020	(2)
PUBTNS	1.0000	(30)	0.9988	(2)	0.9989	(2)
FLATPU	1.0000	(30)	0.9996	(2)	0.9991	(2)
THOR	1.0000	(5)	0.9980	(2)**	0.9978	(2)***
PUSH2O	1.0000	(10)	1.0000	(2)	1.0004	(2)
HISHPG	1.0000	(110)	1.0117	(2)*	1.0075	(2)
PNL2	1.0000	(65)	1.0043	(4)	1.0014	(4)
PNL33	1.0024	(21)	1.0066	(2)*	1.0054	(2)*

Table D-2. Differences for VALIDATION_CRITICALITY Suite

Benchmark = Benchmark values from experiments
621_71_mac = mcnp6.2.1 + Intel-18 + endf/b-vii.1 + macos
621_80_mac = mcnp6.2.1 + Intel-18 + endf/b-viii.0 + macos

Differences are relative to reference case: Benchmark
*'s indicate differences > 1, 2, or 3 std

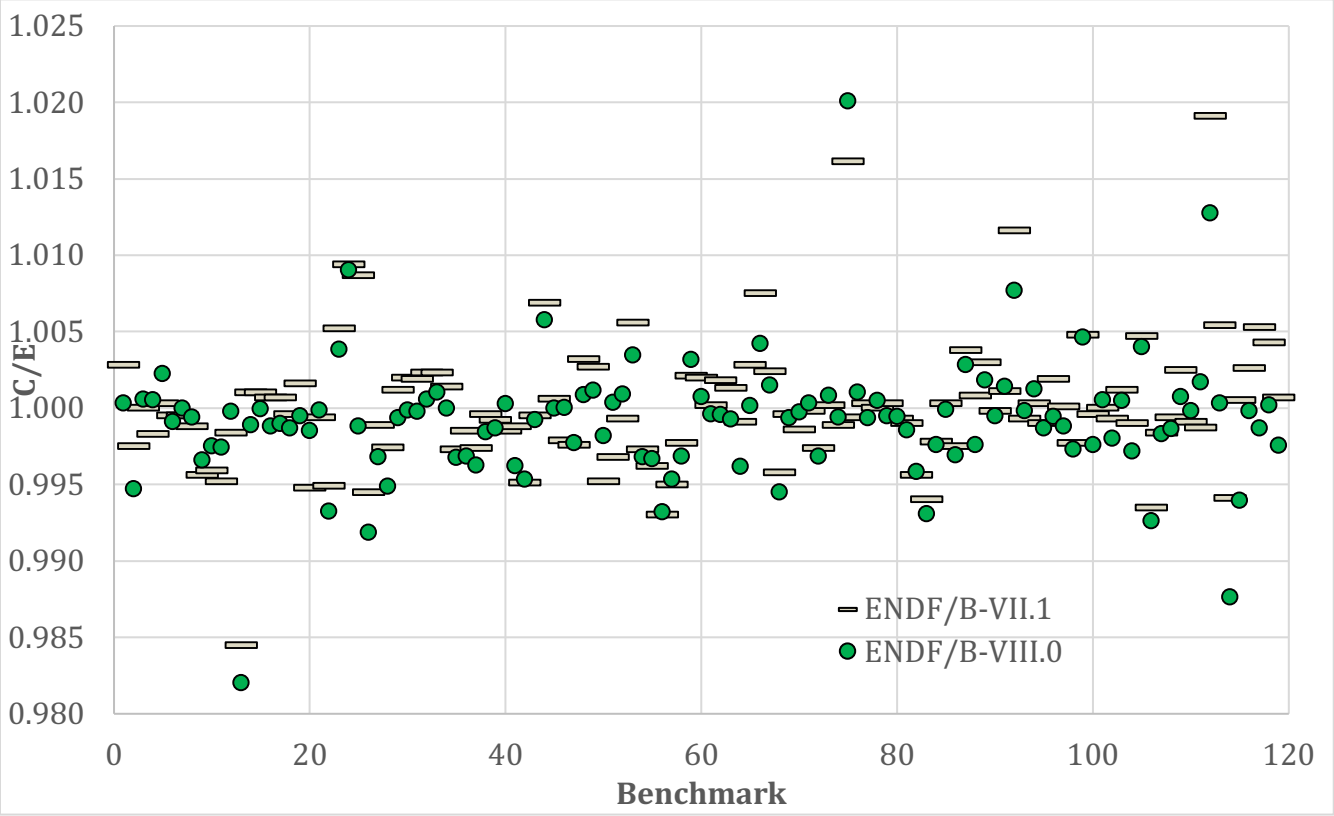
	Benchmark keff std	621_71_mac deltak std	621_80_mac deltak std
U233 Benchmarks			
JEZ233	1.0000 (10)	0.0001 (10)	0.0004 (10)
FLAT23	1.0000 (14)	-0.0014 (14)	0.0000 (14)
UMF5C2	1.0000 (30)	-0.0047 (30)*	-0.0026 (30)
FLSTF1	1.0000 (83)	-0.0149 (83)*	-0.0186 (83)**
SB25	1.0000 (23)	0.0011 (24)	0.0001 (24)
ORNL11	1.0006 (28)	0.0009 (29)	-0.0010 (29)
HEU Benchmarks			
GODIVA	1.0000 (10)	0.0003 (10)	-0.0001 (10)
TT2C11	1.0000 (38)	0.0006 (38)	-0.0012 (38)
FLAT25	1.0000 (30)	0.0037 (30)*	0.0013 (30)
GODIVR	0.9985 (11)	0.0014 (11)*	0.0011 (11)
UH3C6	1.0000 (47)	-0.0047 (47)	-0.0018 (47)
ZEUS2	0.9997 (8)	-0.0034 (8)***	-0.0003 (8)
SB5RN3	1.0015 (28)	-0.0059 (28)**	-0.0080 (28)**
ORNL10	1.0015 (26)	-0.0023 (26)	-0.0033 (26)*
IEU Benchmarks			
IMF03	1.0000 (17)	0.0030 (17)*	-0.0001 (17)
BIGTEN	0.9948 (13)	-0.0003 (13)	-0.0005 (13)
IMF04	1.0000 (30)	0.0076 (30)**	0.0053 (30)*
ZEBR8H	1.0300 (25)	-0.0109 (25)***	-0.0070 (25)**
ICT2C3	1.0017 (44)	0.0023 (44)	0.0029 (44)
STACY36	0.9988 (13)	0.0001 (13)	-0.0004 (13)
LEU Benchmarks			
BAWXI2	1.0007 (11)	0.0001 (12)	0.0001 (12)
LST2C2	1.0024 (37)	-0.0064 (37)*	-0.0065 (37)*
Pu Benchmarks			
JEZPU	1.0000 (20)	-0.0005 (20)	-0.0002 (20)
JEZ240	1.0000 (20)	-0.0001 (20)	0.0020 (20)
PUBTNS	1.0000 (30)	-0.0012 (30)	-0.0011 (30)
FLATPU	1.0000 (30)	-0.0004 (30)	-0.0009 (30)
THOR	1.0000 (5)	-0.0020 (6)**	-0.0022 (6)***
PUSH2O	1.0000 (10)	0.0000 (10)	0.0004 (10)
HISHPG	1.0000(110)	0.0117(110)*	0.0075(110)
PNL2	1.0000 (65)	0.0043 (65)	0.0014 (65)
PNL33	1.0024 (21)	0.0042 (21)*	0.0030 (21)*

Appendix E. Detailed results for VALIDATION_CRIT_EXTENDED benchmark suite

Table E-1. Summary of VALIDATION_CRIT_EXTENDED Suite – 119 ICSBEP cases

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
VALIDATION_CRIT_EXTENDED	119	0.42	0.9994	0.0039	0.41	0.9986	0.0038

Figure E-1. C/E results for Validation_crit_extended Suite using ENDF/B-VII.1 and ENDF/B-VIII.0



Appendix F. Detailed results for Whisper benchmark suite

Table F-1. Summary of results for Whisper benchmark suite using ENDF/B-VII.1 and ENDF/B-VIII.0

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER	1101	0.74	1.0017	0.0072	0.76	1.0003	0.0076
WHISPER: Pu	262	0.97	1.0062	0.0075	0.95	1.0035	0.0088
WHISPER: HEU	386	0.57	1.0016	0.0055	0.63	1.0009	0.0057
WHISPER: MIX	73	0.70	1.0035	0.0060	0.61	1.0018	0.0058
WHISPER: IEU	13	0.43	1.0024	0.0038	0.32	1.0005	0.0033
WHISPER: LEU	209	0.28	0.9995	0.0028	0.28	0.9994	0.0027
WHISPER: ^{233}U	158	1.06	0.9964	0.0100	1.18	0.9939	0.0102

Figure F-1 C/E distribution for Whisper benchmark suite using ENDF/B-VII.1 and ENDF/B-VIII.0

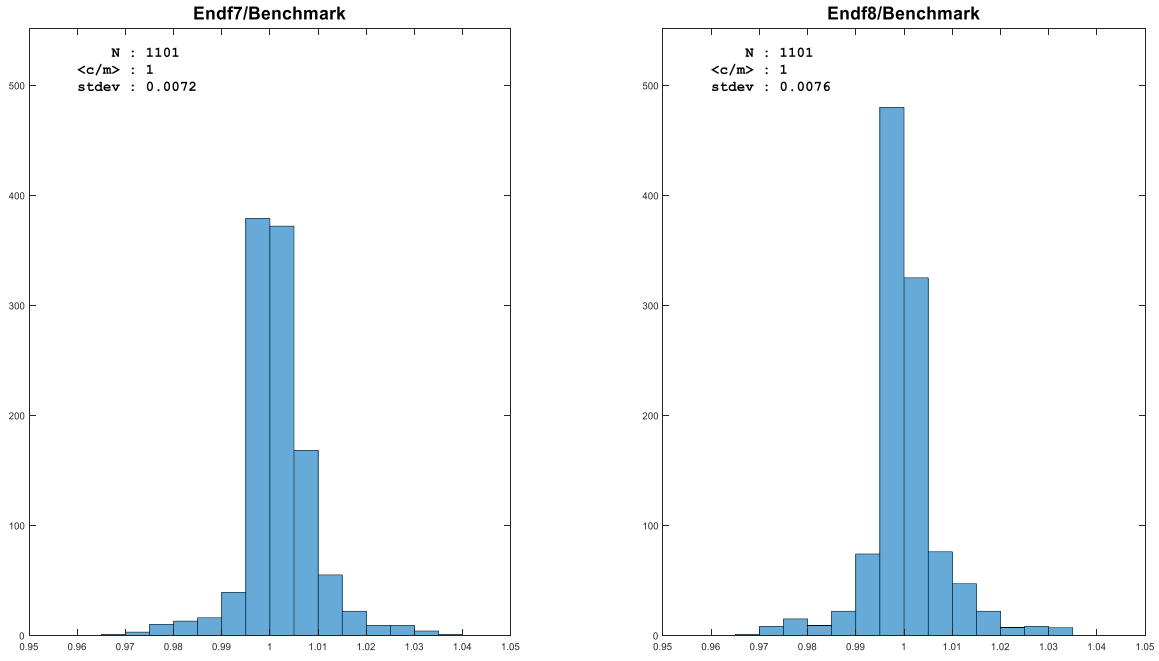


Figure F-2. C/E results for Whisper benchmark suite using ENDF/B-VII.1 and ENDF/B-VIII.0

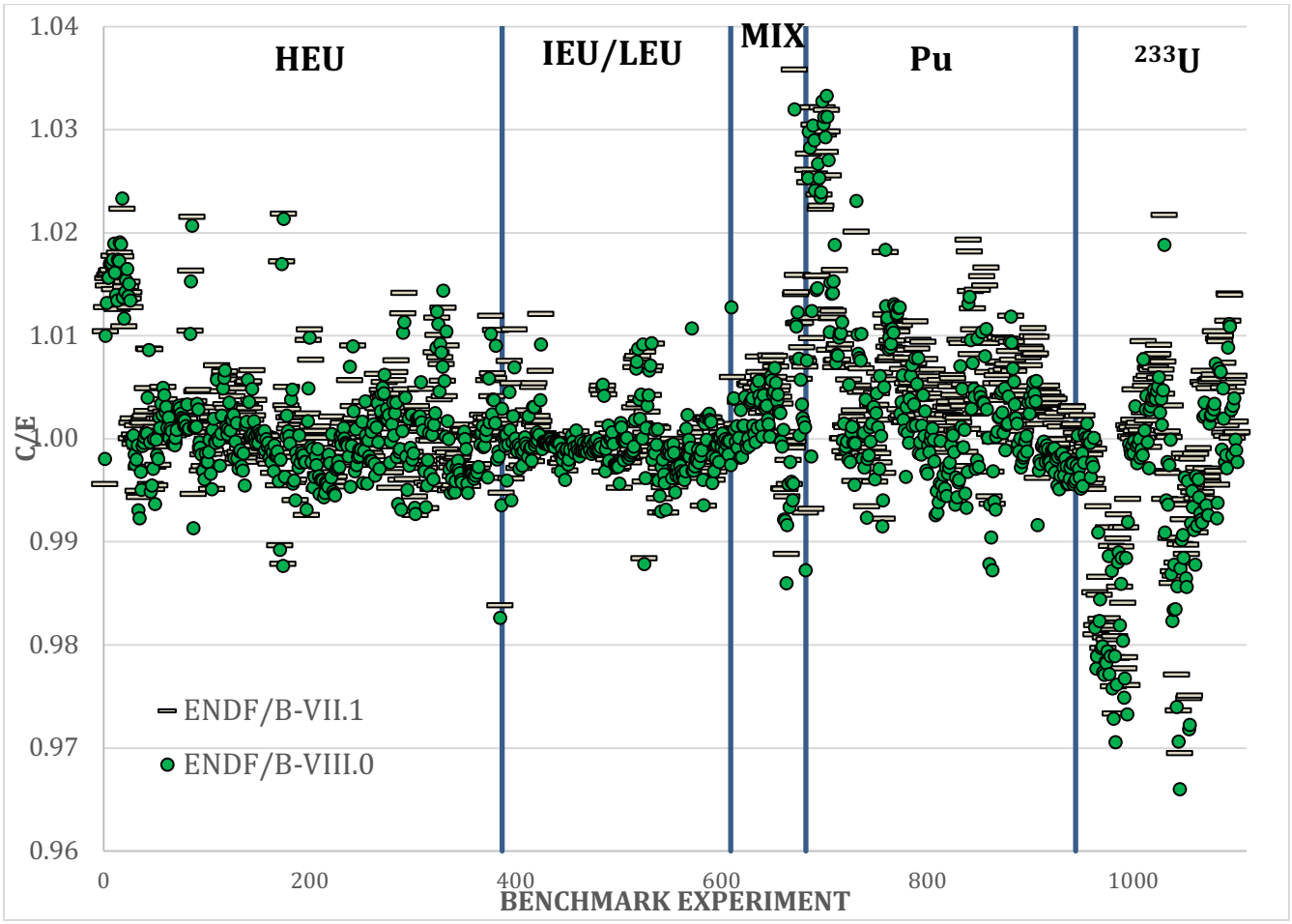


Table F-2. Summary of results for Whisper suite – 262 Pu cases using ENDF/B-VII.1 and ENDF/B-VIII.0

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: Pu	**262**	**0.97**	**1.0062**	**0.0075**	**0.95**	**1.0035**	**0.0088**
WHISPER: PU-COMP	36	2.06	1.0177	0.0106	2.14	1.0186	0.0108
WHISPER: PU-MET	68	0.66	1.0040	0.0054	0.73	1.0039	0.0063
WHISPER: PU-SOL	158	0.64	1.0045	0.0045	0.47	0.9999	0.0047

Figure F-3. C/E results for Whisper suite – 262 Pu cases using ENDF/B-VII.1 and ENDF/B-VIII.0

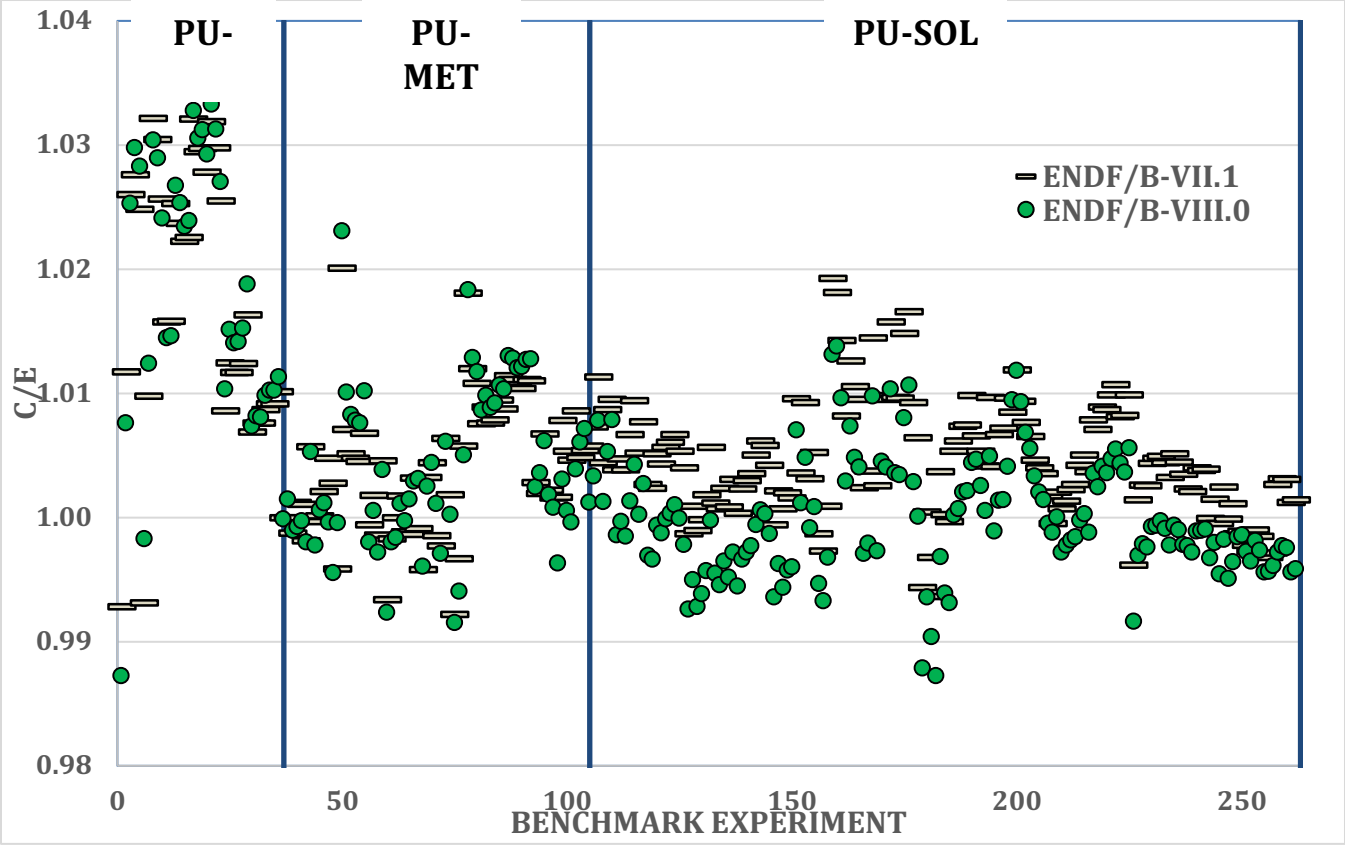


Table F-3. Summary of results for Whisper suite – 386 HEU cases using ENDF/B-VII.1 and ENDF/B-VIII.0

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: HEU	**386**	**0.57**	**1.0016**	**0.0055**	**0.63**	**1.0009**	**0.0057**
WHISPER: HEU-COMP	26	1.50	1.0143	0.0046	1.57	1.0151	0.0044
WHISPER: HEU-MET	267	0.42	1.0009	0.0041	0.40	0.9999	0.0041
WHISPER: HEU-SOL	93	0.47	1.0000	0.0047	0.49	0.9998	0.0049

Figure F-4. C/E results for Whisper suite – 386 HEU cases using ENDF/B-VII.1 and ENDF/B-VIII.0

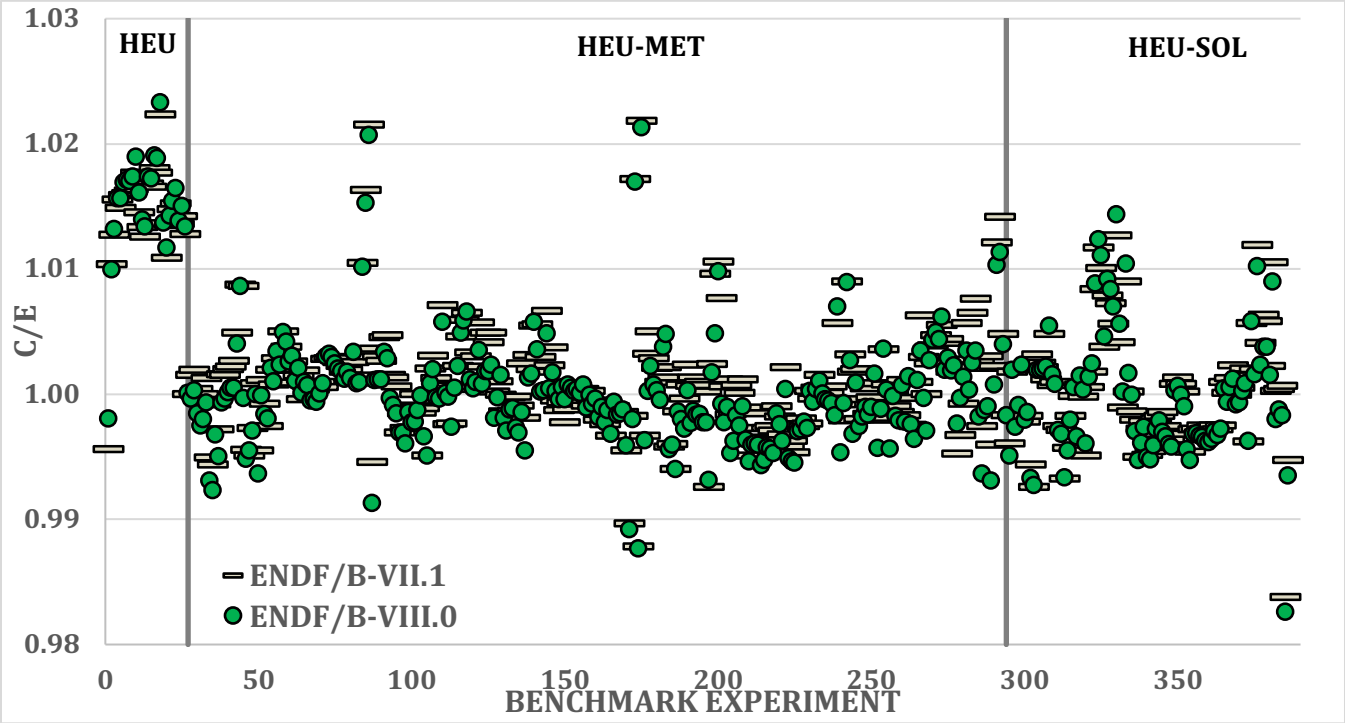


Table F-4. Summary of results for Whisper suite – 295 IEU, LEU, MIX cases using ENDF/B-VII.1 and ENDF/B-VIII.0

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: MIX	73	0.70	1.0035	0.0060	0.61	1.0018	0.0058
WHISPER: IEU	13	0.43	1.0024	0.0038	0.32	1.0005	0.0033
WHISPER: LEU	209	0.28	0.9995	0.0028	0.28	0.9994	0.0027

Figure F-5. C/E results for Whisper suite – 295 IEU, LEU, MIX cases using ENDF/B-VII.1 and ENDF/B-VIII.0

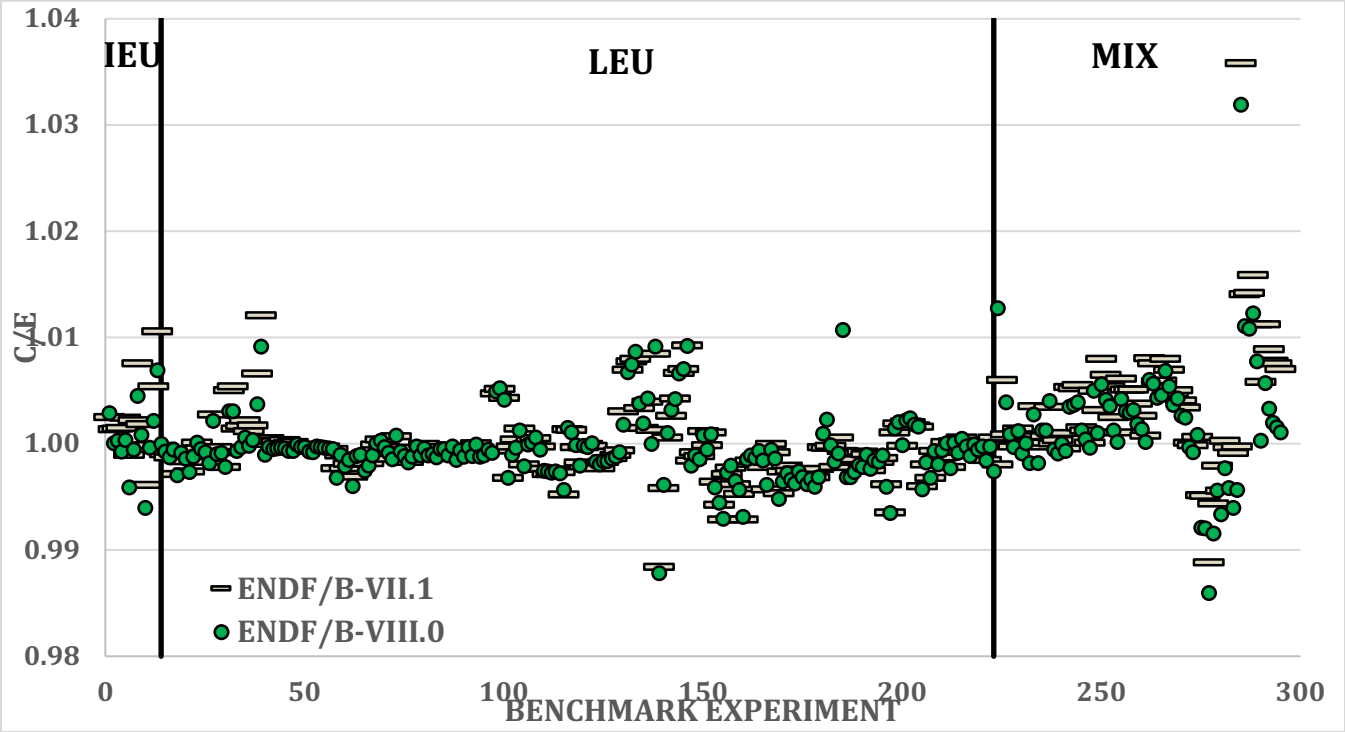


Table F-5. Summary of results for Whisper suite – 158 U-233 cases using ENDF/B-VII.1 and ENDF/B-VIII.0

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: ^{233}U	**158**	**1.06**	**0.9964**	**0.0100**	**1.18**	**0.9939**	**0.0102**
WHISPER: ^{233}U: COMP-THERM	9	0.20	0.9995	0.0020	0.33	0.9971	0.0016
WHISPER: ^{233}U: MET-FAST	10	0.25	0.9982	0.0019	0.17	0.9993	0.0017
WHISPER: ^{233}U: SOL-INTER	33	1.72	0.9837	0.0056	1.99	0.9809	0.0056
WHISPER: ^{233}U: SOL-THERM	106	0.87	0.9999	0.0087	0.92	0.9971	0.0088

Figure F-6. C/E results for Whisper suite – 158 U-233 cases using ENDF/B-VII.1 and ENDF/B-VIII.0