Title: Impact of Outliers and ENDF/B-VIII.0 on NCS Validation and USLs

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Review**

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Impact of Outliers and ENDF/B-VIII.0 on
NCS Validation and USLs

Jennifer Alwin   &   Forrest Brown

Comparison of Benchmarks and Applications

- **Goal**
  - **Determine impact of rejection of benchmark outliers on NCS validation**
  - **Identify benchmark outliers in Whisper-1.1 using ENDF/B-VIII.0 vs. ENDF/B-VII.1**
  - **Compare ENDF/B-VIII.0 for criticality safety calculations relative to previous, mostly ENDF/B-VII.1,for various criticality validation suites and some applications.**
    - **Benchmarks from ICSBEP handbook Pu, HEU, LEU, IEU, MIX, ^{233}U**
    - **Thermal, intermediate, fast and mixed spectrum**
    - **Calculational results compared with ICSBEP results for benchmarks**
- **ENDF/B-VIII.0**
  - **N sub library**
  - **CIELO evaluations: ^{1}H, ^{16}O, ^{56}Fe, ^{235}U, ^{238}U, ^{239}Pu, PFNS, PFGS**
  - **New light elements n, ^{2}H, ^{3}He, ^{6}Li, ^{9}Be, ^{10}B, ^{12,13}C, ^{35,37}Cl, ^{18}O**
  - **^{40}Ca, ^{54,56,57,58}Fe, $^{58-62,64}$Ni, ^{59}Co, ^{63,65}Cu, $^{174-182}$Hf, $^{182-186}$W, ^{105}Rh, ^{132}Te**
  - **New ^{236m}Np, ^{240}Pu nubar, revised ^{241,243}Am**
  - **TSL**
  - **Fuels: UO_2, UN**
  - **Moderators: water, graphite, poly, lucite, yttrium hydride**
  - **Reflectors: Be, BeO**
  - **Natural: ice, SiO_2**
  - **Cladding, SiC**

Benchmark Outlier Rejection

- ## Whisper Identification of Outliers
    - ### Generalized Linear Least Squares (GLLS)
        - Used to find the minimum chi-squared
        - Value of chi-squared per number of benchmarks should be unity for perfect regression model
        - Rejected using iterative diagonal chi-squared method until $\chi^2 < 1.2$
        - 10% of Whisper-1.1 library identified as outliers using method
        - Whisper computed USL, user option to include identified outliers

- ## Rejection of Outliers
    - ### ANSI/ANS-8.24-2007:
    - *"Rejection of data outliers shall be based on the inconsistency of the data with known physical behavior or on established statistical rejection methods."*
    - ### ANSI/ANS-8.24-2017:
   - **"***Identification of data outliers may be based on established statistical rejection methods; rejection of outliers shall be based on the inconsistency of the data with known physical behavior in the experimental data.*"

Impact of Rejected Benchmarks on Validation

– **Application parameter study models for use with MCNP6/Whisper-1.1**
– **Pu and HEU: metal, oxide, solution**

- **Metal and Oxide**
    - Metal- or oxide- water mixture
    - 3 cylinders
    - Water, steel reflection
    - H/D variation
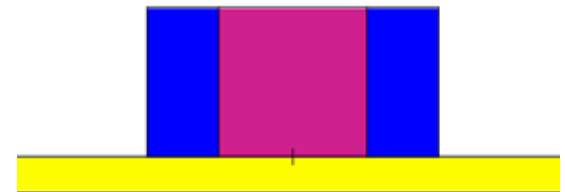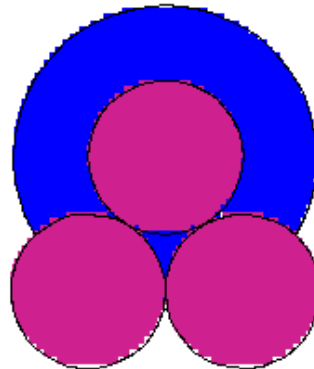
- **Solution**
    - Metal-water mixture
    - 2 cylinders
    - Water, steel reflection
    - H/D variation
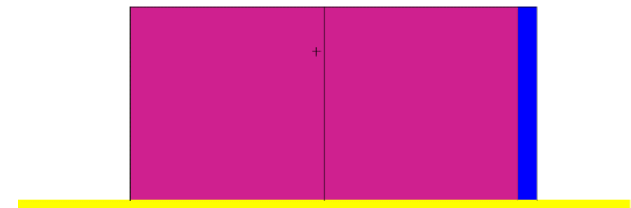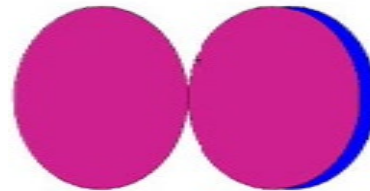
– **MCNP6.2 calculations using 1,000,000 neutrons**
– **Whisper-1.1 calculation of Bias, Bias Uncertainty, MOS → USL**

Results of Benchmark Rejection Study

Pu Metal
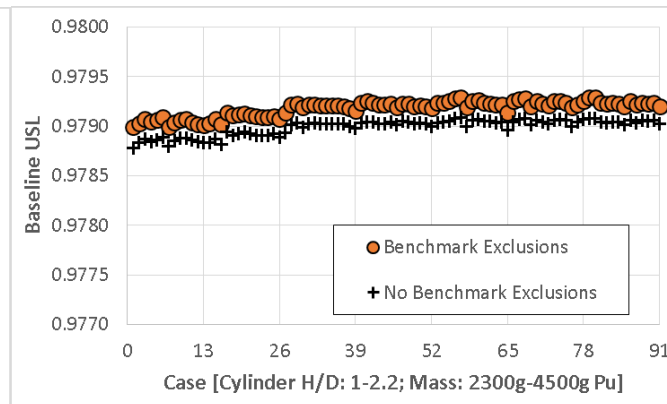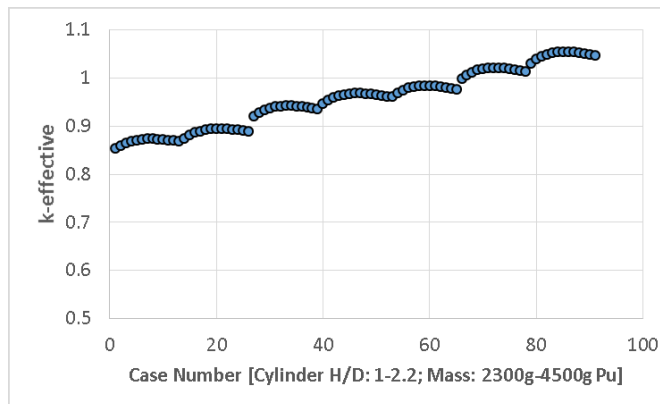
Pu Oxide
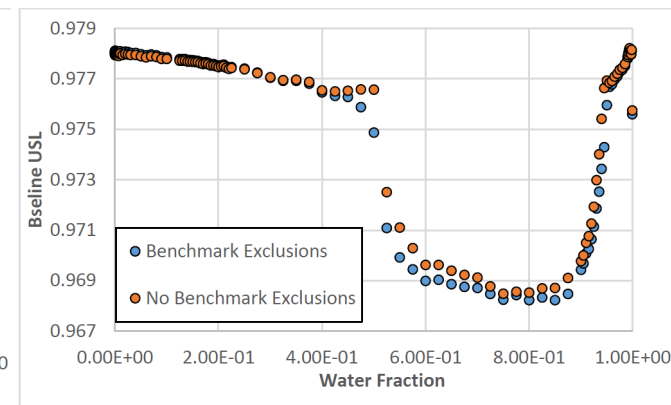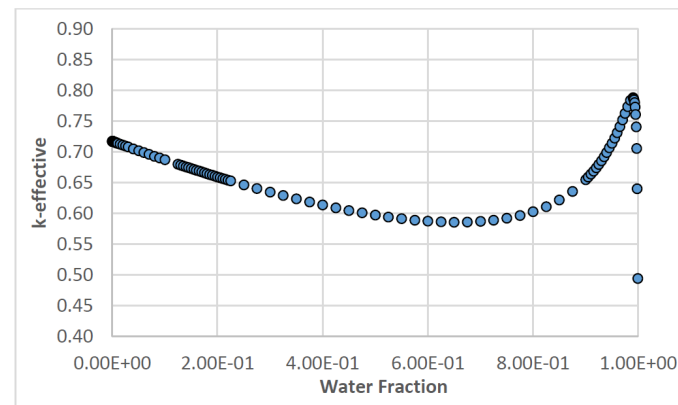
Pu Solution
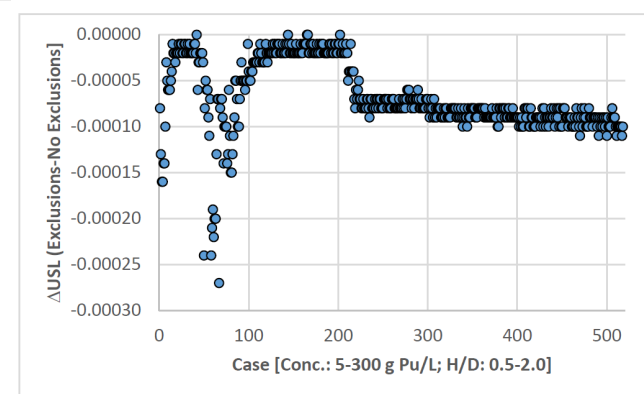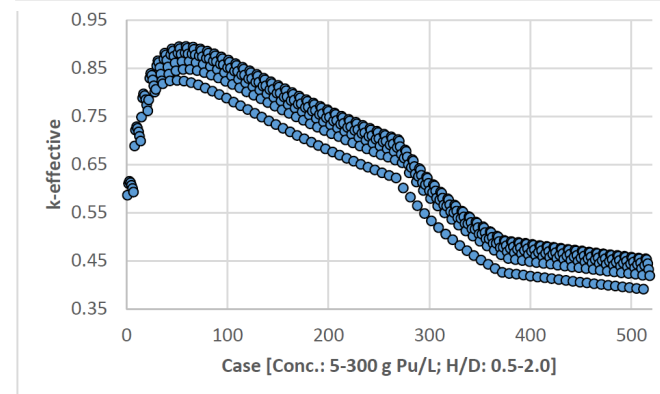
Results of Benchmark Rejection Study

HEU Metal
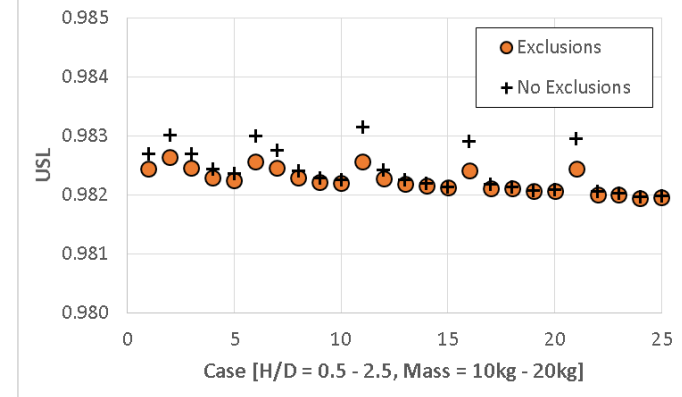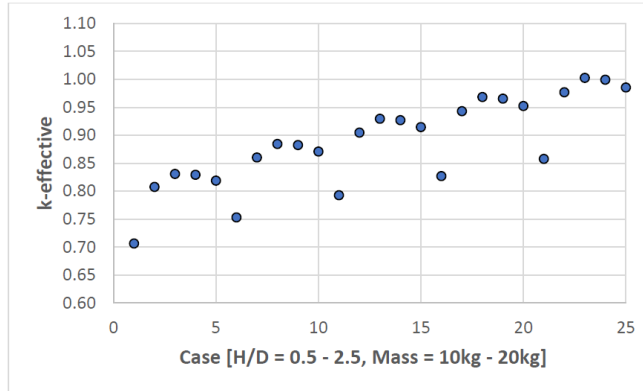
HEU Oxide
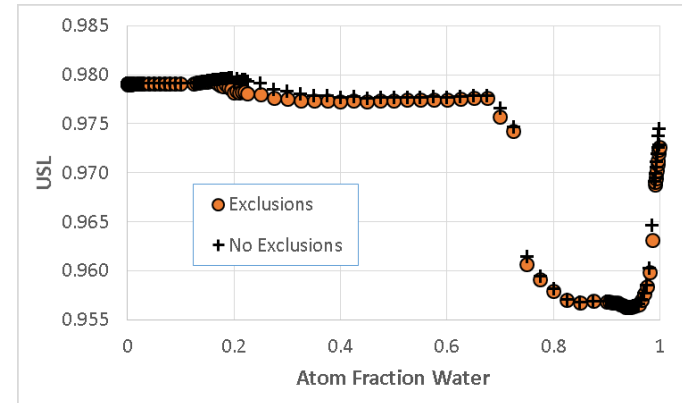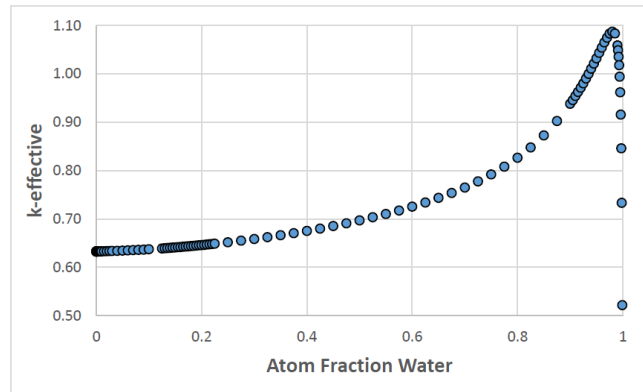
HEU Solution
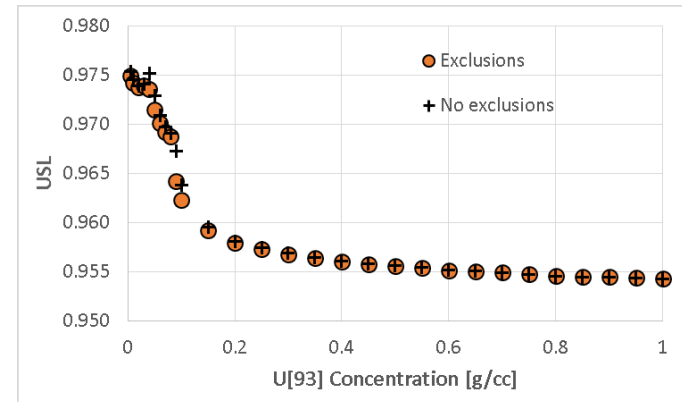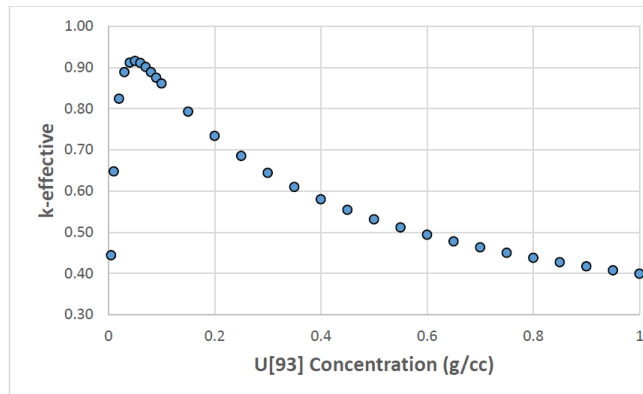
Results of Benchmark Rejection & ENDF/B-VIII.0 Study

Rejection Study USL Differences

- Pu metal =   0.00021
- Pu oxide =   0.00234
- Pu solution =   0.00026
- HEU metal =   0.0005
- HEU oxide =   0.00208
- HEU solution = 0.00307
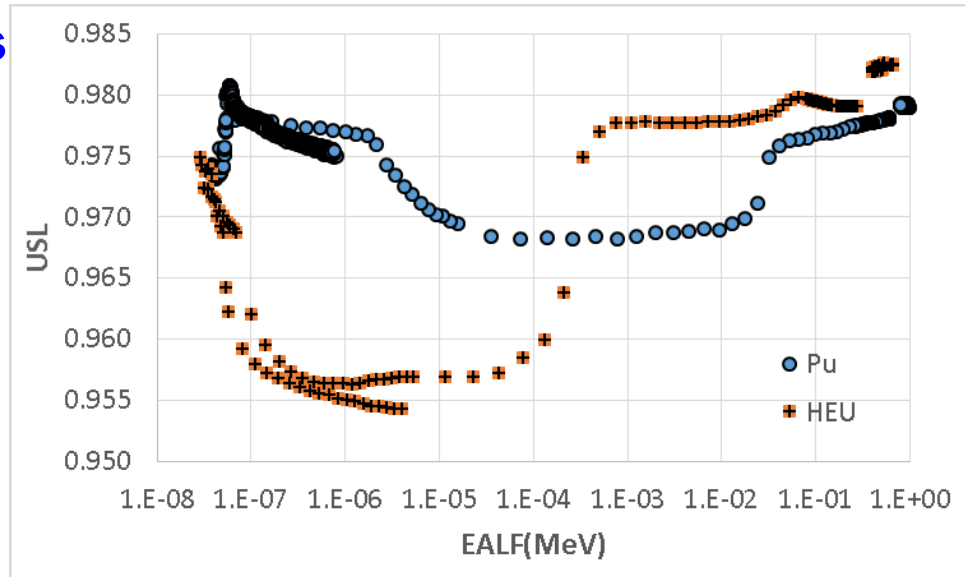
ENDF/B-VII.1 vs. ENDF-B/VIII.0 K-effective Differences

- No values for experiment; plot is Δ k-effective –VIII.0 & –VII.1 as function of lethargy

- Lower k-effective in thermal Pu: correction of over prediction prior to –VIII.0
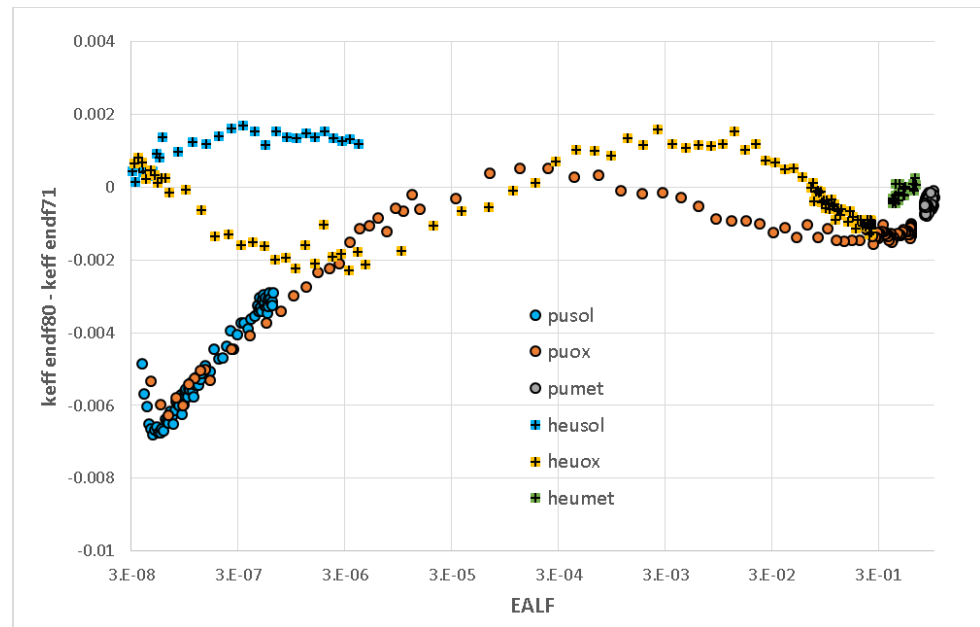
Rejected Benchmarks Identified with Whisper

– Outliers found over a range of materials and energy spectra

– Fewer outliers using ENDF/B-VIII.0 than ENDF/B-VII.1

Benchmark Series	# Library	Rejected- ENDF/B-VII.1	% Library	Rejected- ENDF/B-VIII.0	% Library
HEU-COMP-THERM	25	5	20%	3	12%
HEU-MET-FAST	251	29	12%	26	10%
HEU-MET-INTER	4	2	50%	1	25%
HEU-MET-THERM	4	2	50%	2	50%
HEU-SOL-THERM	93	2	2%	0	0%
LEU-COMP-THERM	182	4	2%	3	2%
LEU-SOL-THERM	27	2	7%	2	7%
MIX-MET-FAST	32	1	3%	1	3%
MIX-SOL-THERM	21	9	43%	9	43%
PU-COMP-MIXED	34	16	47%	15	44%
PU-MET-FAST	68	3	4%	2	3%
PU-SOL-THERM	158	15	9%	13	8%
U233-MET-FAST	9	1	11%	1	11%
U233-SOL-INTER	33	10	30%	9	27%
U233-SOL-THERM	106	12	11%	11	10%
OTHER	54	0	0%	0	0%
TOTAL	1101	113	10%	98	9%

Results of Validation_Criticality 31 problems

- ## Results
  - **Good agreement with both ENDF-B-VII.1 and ENDF/B-VIII.0 nuclear data libraries**

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
VAL_CRIT	**31**	**0.56**	**0.9999**	**0.0057**	**0.59**	**0.9989**	**0.0059**
233U	7	0.66	0.9962	0.0058	0.74	0.9956	0.0065
HEU	7	0.22	0.9994	0.0023	0.19	0.9987	0.0014
IEU	6	0.76	1.0029	0.0083	0.87	1.0027	0.0099
LEU	2	0.47	0.9975	0.0055	0.47	0.9970	0.0050
Pu	9	0.50	1.0018	0.0046	0.33	1.0004	0.0032

Benchmark		k-eff ex.	k-eff ENDF/B-VII.1	k-eff ENDF/B-VIII.0	ENDF/B-VII.1 C/E	ENDF/B-VIII.0 C/E
233U	FLAT23	1.0000	0.9974	0.9978	0.9974	0.9978
	FLSTF1	1.0000	0.9845	0.9819	0.9845	0.9819
	JEZ233	1.0000	1.0000	1.0007	1.0000	1.0007
	ORNL11	1.0006	1.0018	0.9994	1.0012	0.9988
	SB25	1.0000	1.0007	1.0000	1.0007	1.0000
	UMF5C2	1.0000	0.9960	0.9969	0.9960	0.9969
HEU	SB5RN3	1.0015	0.9954	0.9949	0.9939	0.9934
	FLAT25	1.0000	1.0034	0.9999	1.0034	0.9999
	GODIVA	1.0000	0.9988	0.9990	0.9988	0.9990
	GODIVR	0.9985	0.9989	0.9979	1.0004	0.9994
	ORNL10	1.0015	1.0001	0.9981	0.9986	0.9966
	TT2C11	1.0000	1.0009	0.9988	1.0009	0.9988
	UH3C6	1.0000	0.9965	0.9969	0.9965	0.9969
	ZEUS2	1.0001	0.9976	1.0006	0.9975	1.0004
IEU	BIGTEN	1.0045	0.9952	0.9948	0.9908	0.9904
	ICT2C3	1.0017	1.0035	1.0036	1.0018	1.0019
	IMF03	1.0000	1.0019	0.9988	1.0019	0.9988
	IMF04	1.0000	1.0082	1.0052	1.0082	1.0052
	STACY36	0.9988	0.9981	0.9987	0.9993	0.9999
	ZEBR8H	1.0030	1.0185	1.0232	1.0155	1.0201
LEU	BAWXI2	1.0007	1.0021	1.0012	1.0013	1.0005
	LST2C2	1.0024	0.9960	0.9958	0.9936	0.9935
Pu	FLATPU	1.0000	1.0004	0.9981	1.0004	0.9981
	HISHPG	1.0000	1.0121	1.0078	1.0121	1.0078
	JEZ240	1.0000	0.9999	1.0014	0.9999	1.0014
	JEZPU	1.0000	0.9990	0.9996	0.9990	0.9996
	PNL2	1.0000	1.0050	0.9990	1.0050	0.9990
	PNL33	1.0024	1.0068	1.0047	1.0043	1.0023
	PUBTNS	1.0000	0.9980	0.9979	0.9980	0.9979
	PUSH2O	1.0000	0.9998	1.0001	0.9998	1.0001
	THOR	1.0000	0.9976	0.9973	0.9976	0.9973

Results of Various Benchmark Suites

- **Results ENDF/B-VIII.0 improved**
  - **Pu**
  - **PU-SOL**
  - **HEU, HEU-MET**
  - **MIX**
  - **IEU**
  - **^{233}U-MET-FAST**
- **Other results not much different**

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**
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: 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
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
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**
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

Results of Validation_Crit_Extended, 119 cases

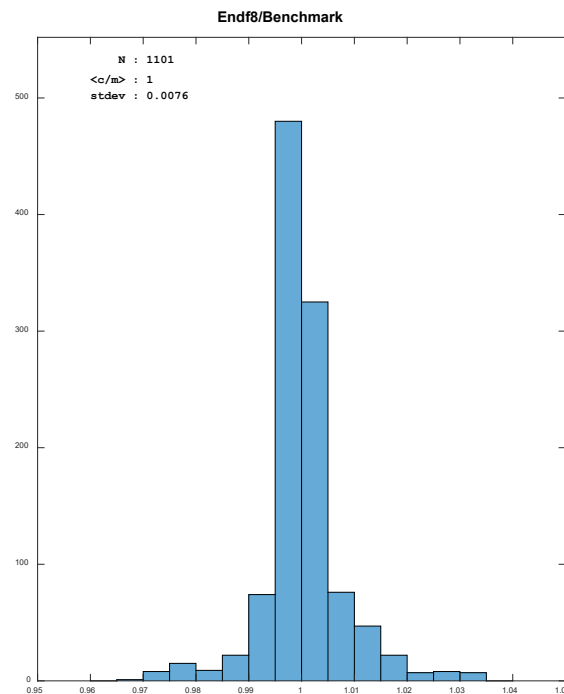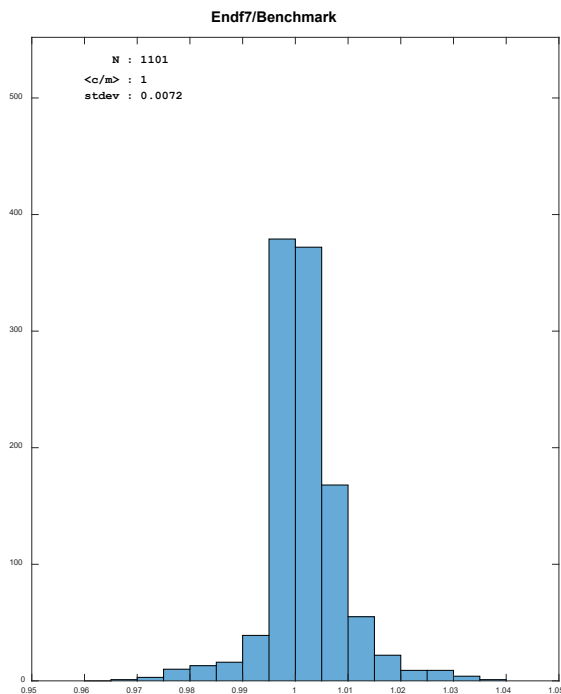| Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
VALIDATION_CRIT_EXTENDED	119	0.42	0.9994	0.0039	0.41	0.9986	0.0038
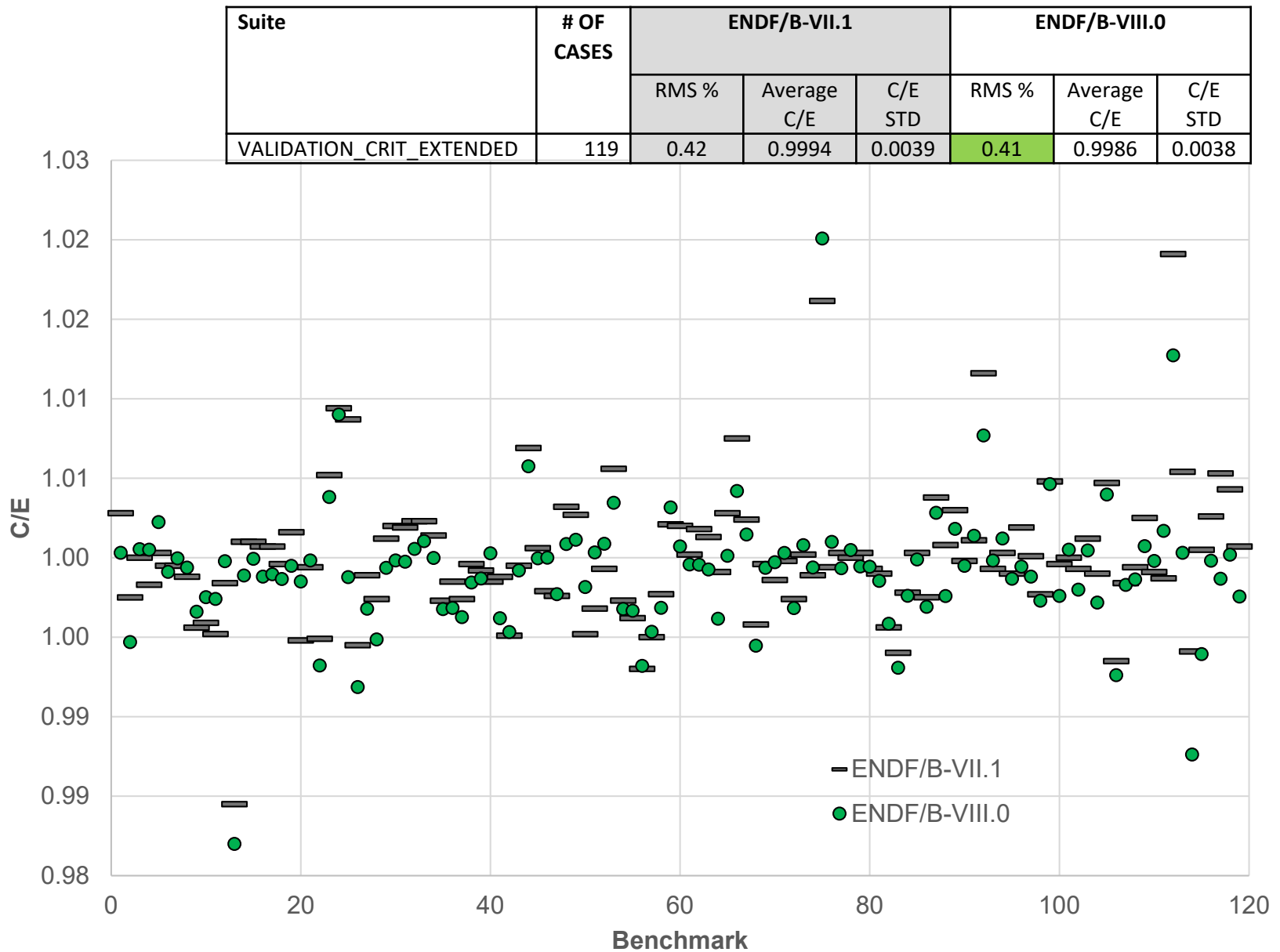
Results of Whisper Library, 1101 cases
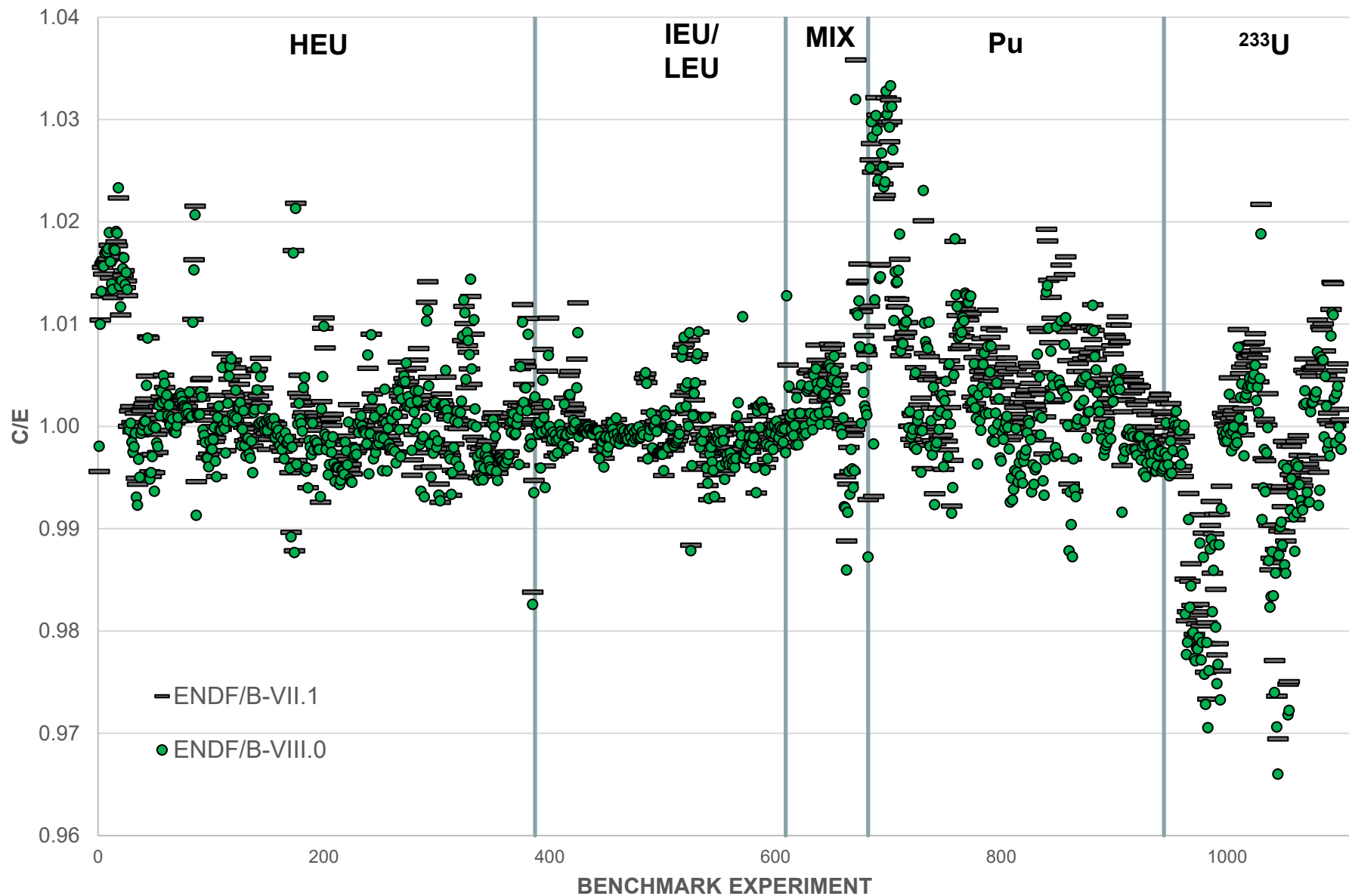
- ## ENDF/B-VIII.0

  – **Large benchmark set**
  – **Good performance, higher std.**
  – **Agreement with results in Nuclear Data Sheets[1]**

  D. A. Brown, et. al, "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data", Nuclear Data Sheets 148 (2018) 1-142

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

Endf7/Benchmark

N : 1101
<c/m> : 1
stdev : 0.0072

Endf8/Benchmark

N : 1101
<c/m> : 1
stdev : 0.0076

Results of Whisper Library, 1101 cases

Results of Whisper Library, 262 Pu cases

- ## Pu results

  - **Improved ENDF/B-VIII.0 for Pu overall and specifically Pu solution**

  - **Pu metal about the same**

  - **Pu compounds not great for –VII.1 or –VIII.0, mixed spectrum**

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

Results of Whisper Library, 36 PU-COMP 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
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

- **Pu results**
  - **PU-COMP highest standard deviation and RMS of Whisper suite**
  - **Mixed and intermediate spectrum**
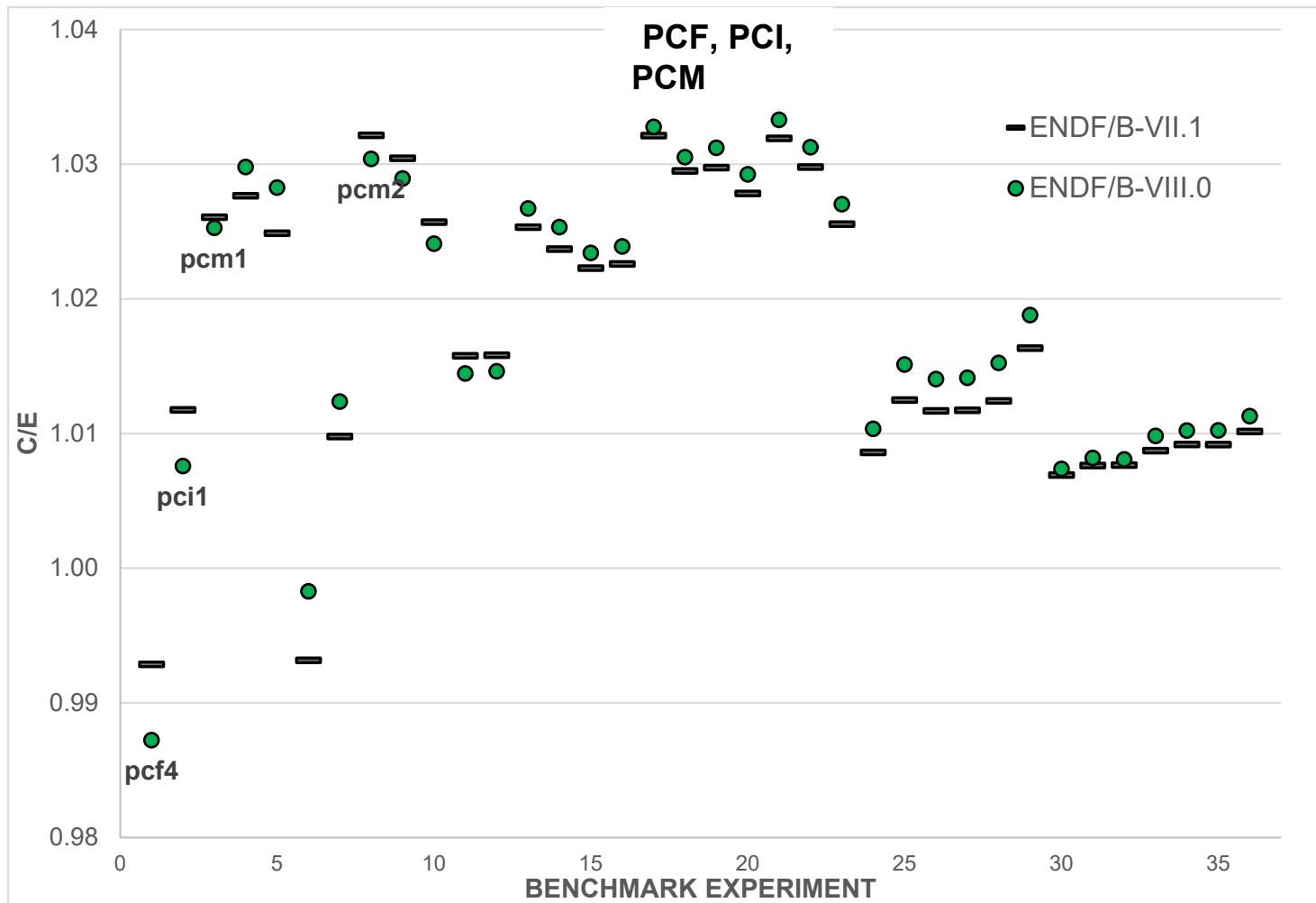
Results of Whisper Library, 68 PMF cases

•Pu results

–**Pu metal slightly better**

–**PMF19,21,38,44: BeO**

–**PMF42: steel**

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-MET	68	0.66	1.0040	0.0054	0.73	1.0039	0.0063
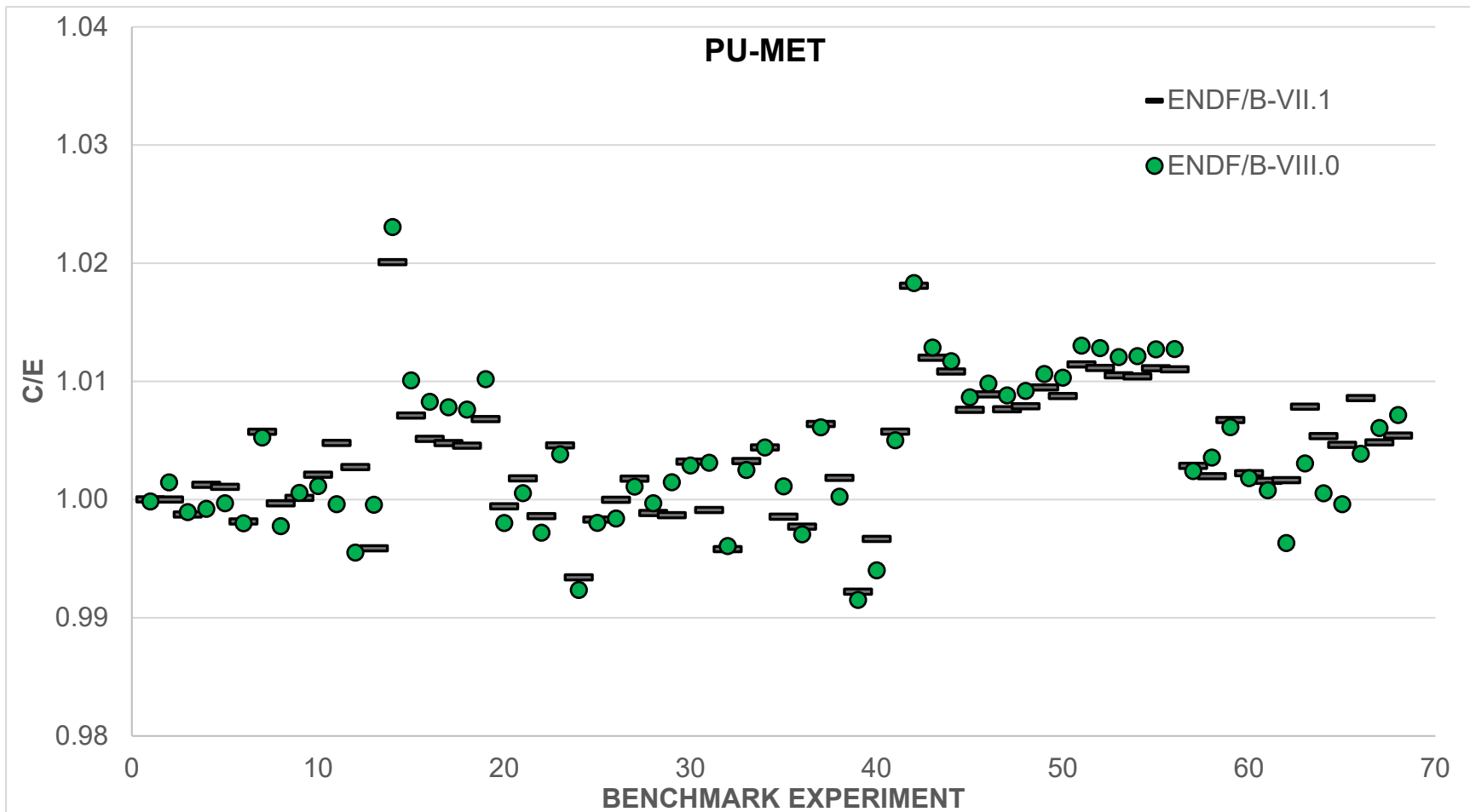
Results of Whisper Library, 158 PST cases

- ## PU-SOL

  - **previously over predicted ~500 pcm**

  - **High experimental uncertainty**

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-SOL	158	0.64	1.0045	0.0045	0.47	0.9999	0.0047
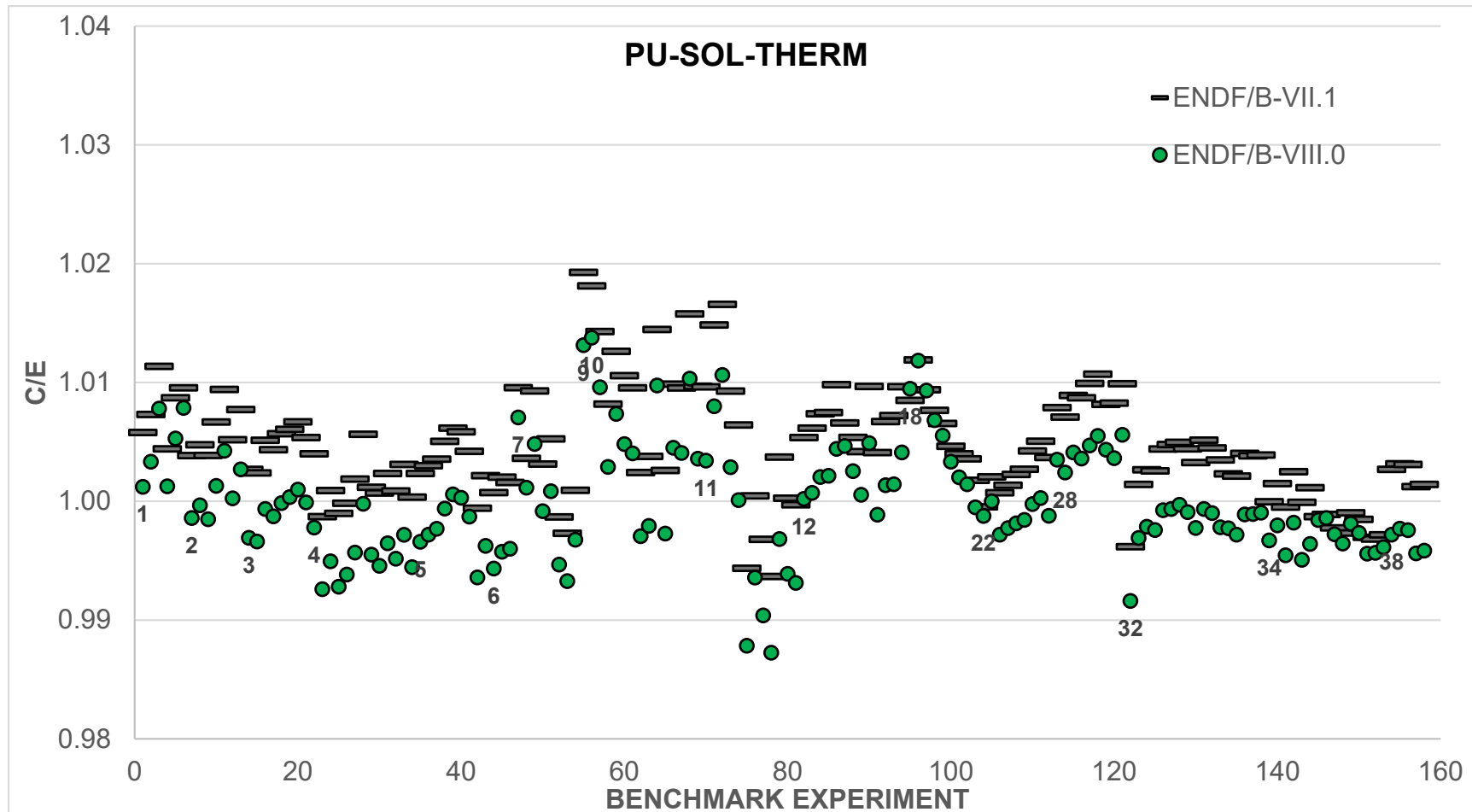
Results of Whisper Library, 386 HEU cases

- ## HEU results

  - **Improved ENDF/B-VIII.0 for HEU, overall, HEU-MET specifically**

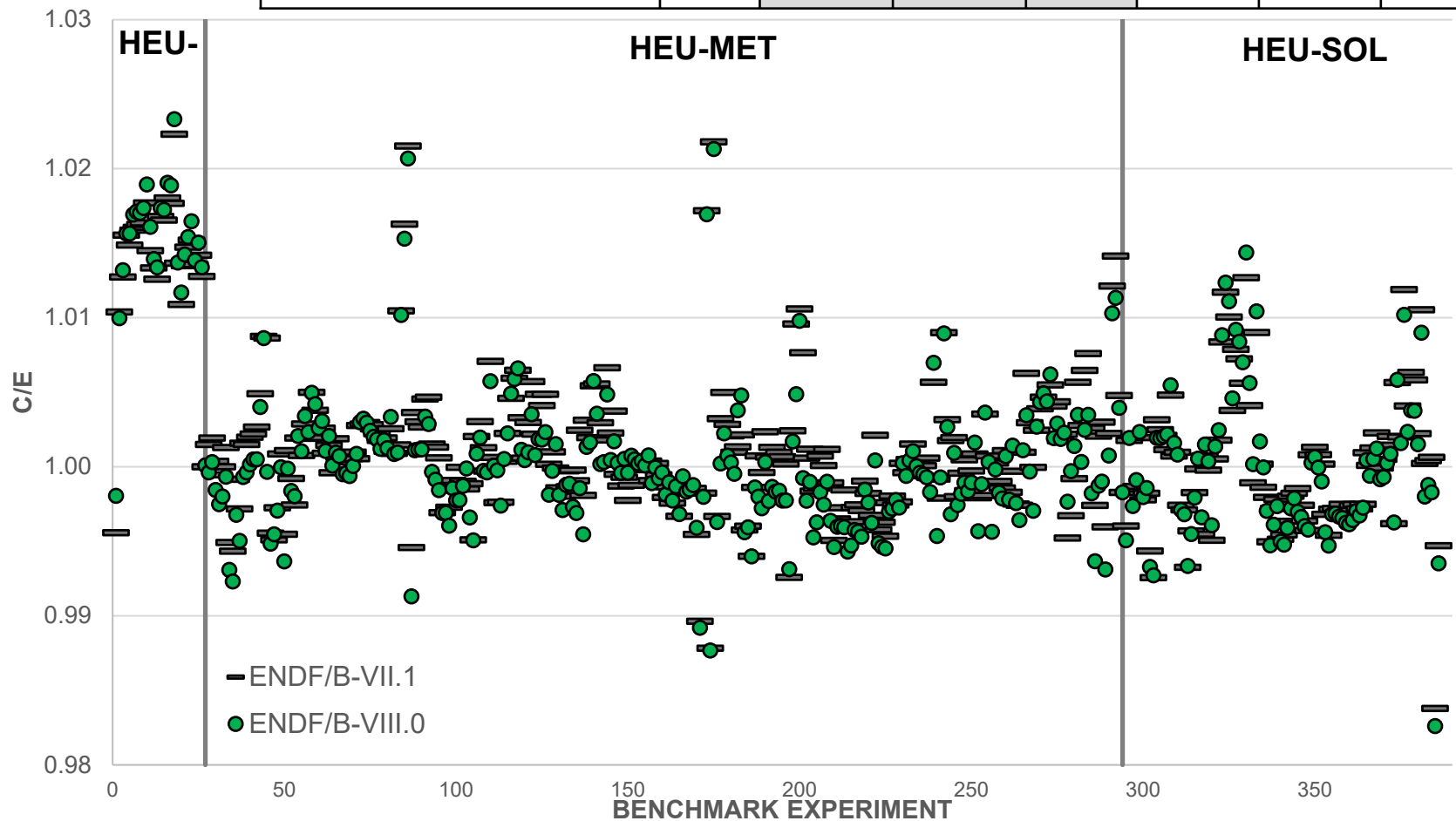| Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: HEU	**386**	**0.57**	**1.0016**	**0.0055**	**0.63**	**1.0009**	**0.0057**
WHISPER: HEU-COMP	26	1.50	1.0143	0.0046	1.57	1.0151	0.0044
WHISPER: HEU-MET	267	0.42	1.0009	0.0041	0.40	0.9999	0.0041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

Results of Whisper Library, 26 HEU-COMP cases

- ## HEU-COMP
  - **Still over predicted**

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
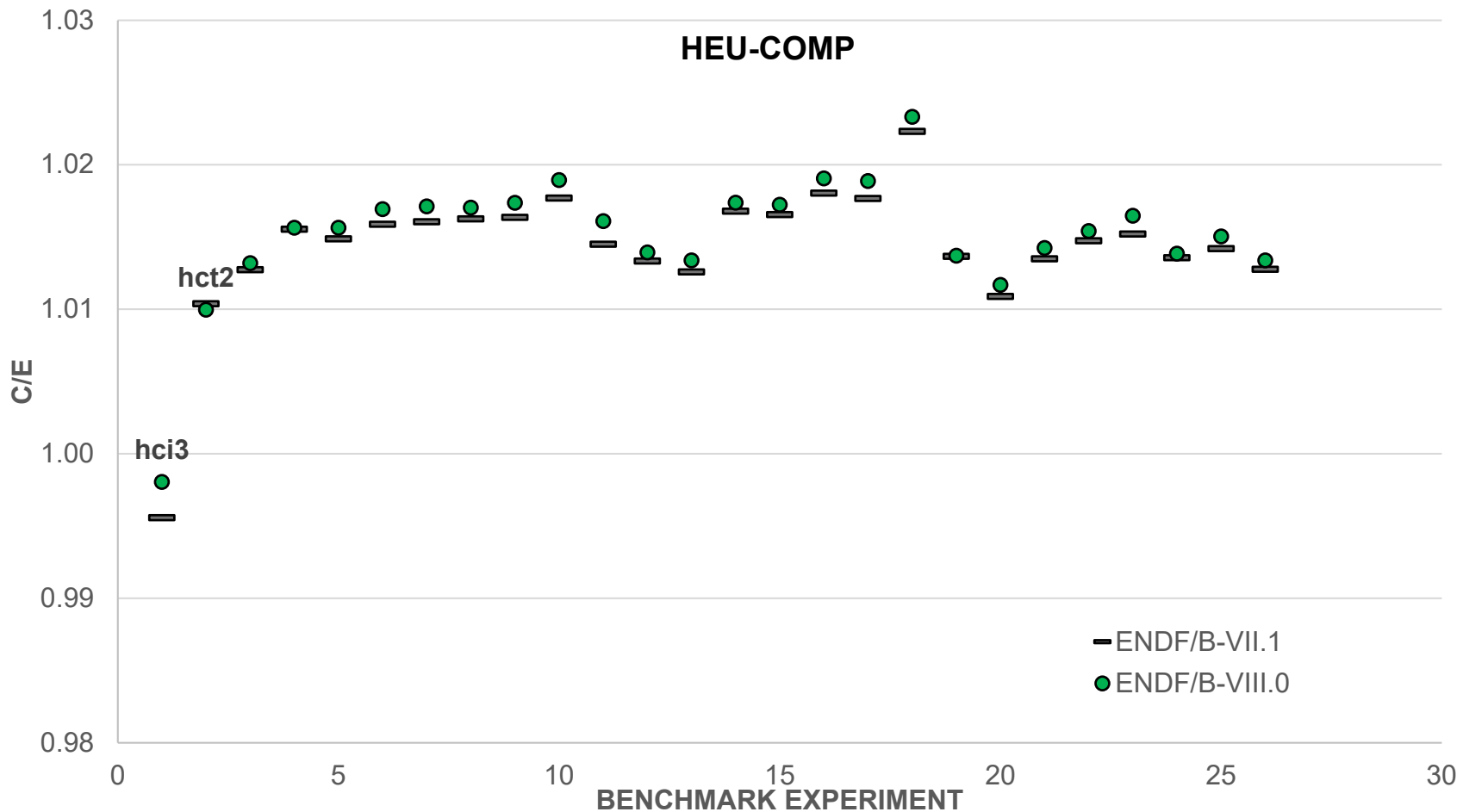
Results of Whisper Library, 267 HEU-MET cases

- ## HEU results
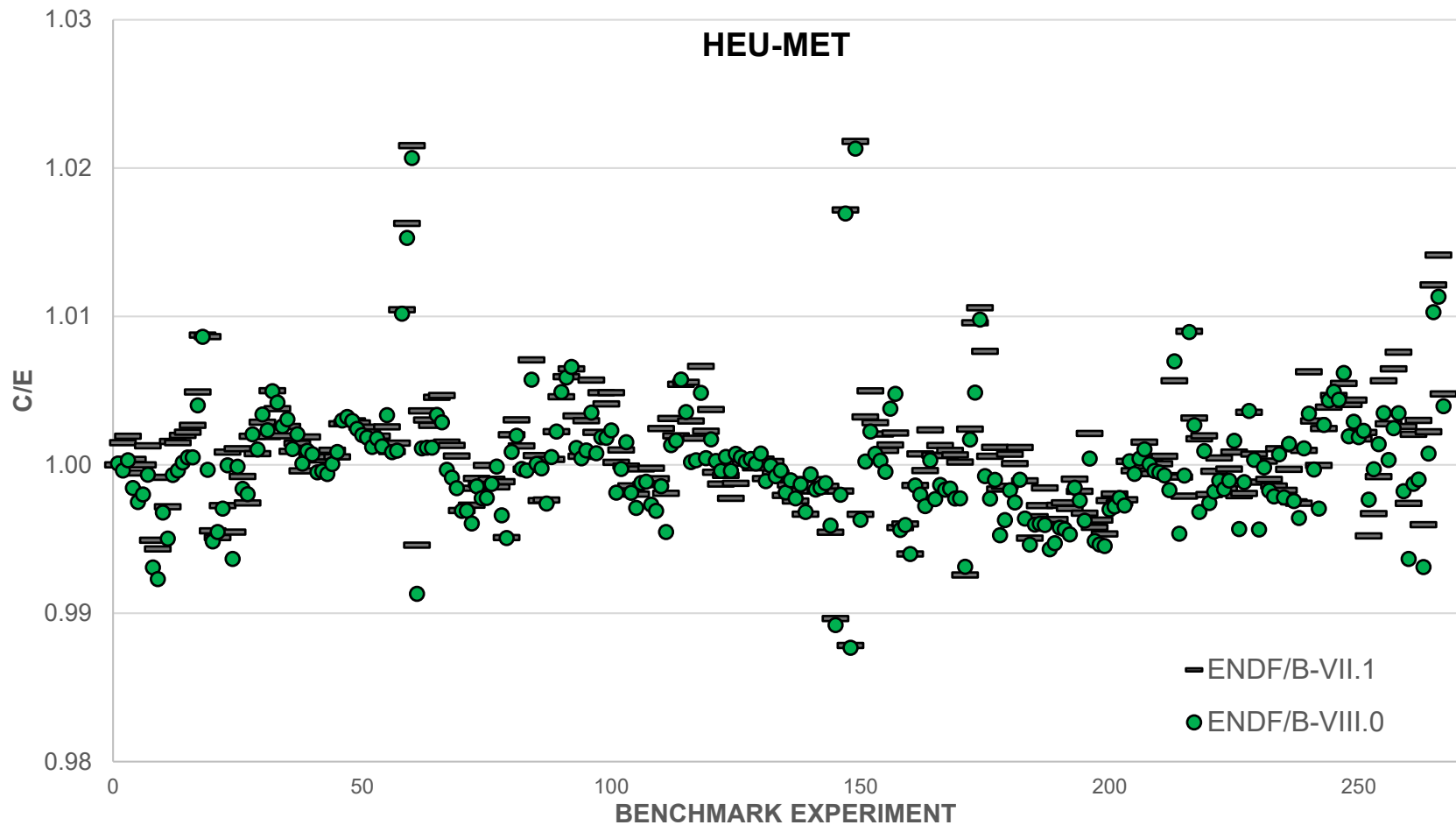 - **Improved ENDF/B-VIII.0 for HEU-MET**
  - **Improved HMF w/ BeO**

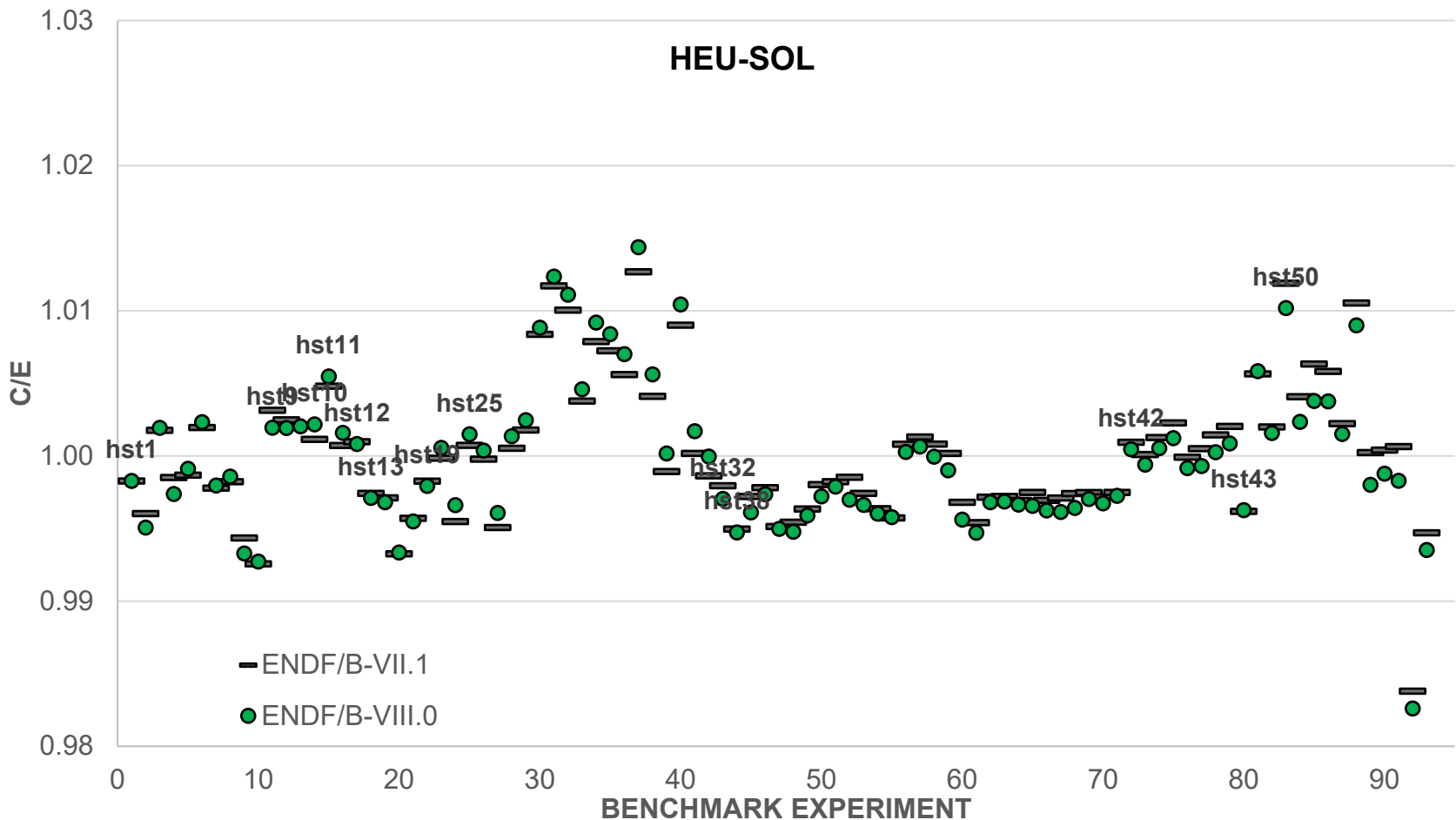| Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: HEU	**386**	**0.57**	**1.0016**	**0.0055**	**0.63**	**1.0009**	**0.0057**
WHISPER: HEU-MET	267	0.42	1.0009	0.0041	0.40	0.9999	0.0041

HEU-MET

Results of Whisper Library, 93 HEU-SOL cases

- ## HST results

  – **Artificially shifted thermal ^{235}U ν, capture, fission data eliminated in –VIII.0**

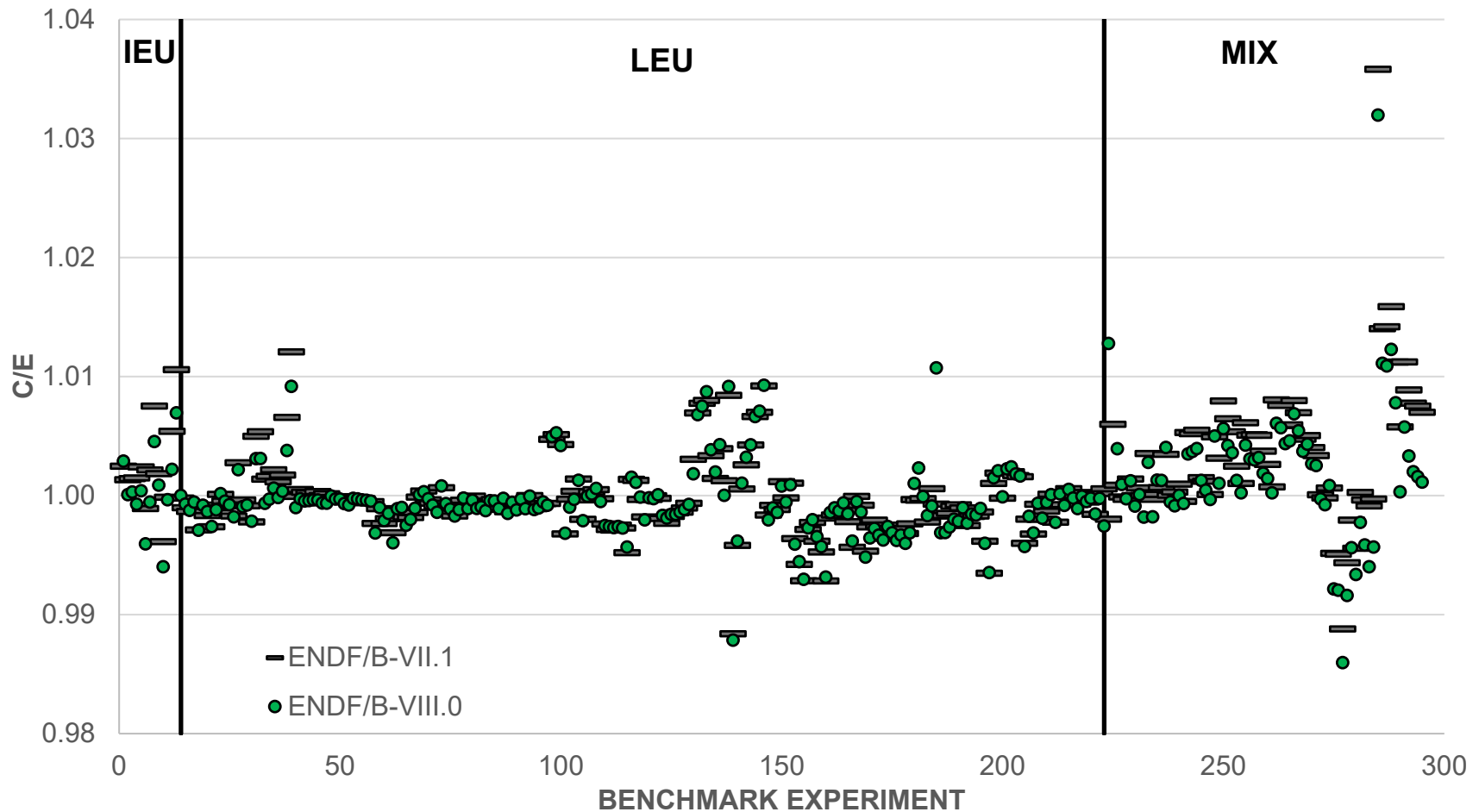| Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: HEU	**386**	**0.57**	**1.0016**	**0.0055**	**0.63**	**1.0009**	**0.0057**
WHISPER: HEU-SOL	93	0.47	1.0000	0.0047	0.49	0.9998	0.0049

Results of Whisper Library, 295 IEU,LEU,MIX cases

• **IEU, LEU, MIX results**

– **Improved ENDF/B-VIII.0 for MIX & IEU**

– **LCT ~same, but good**

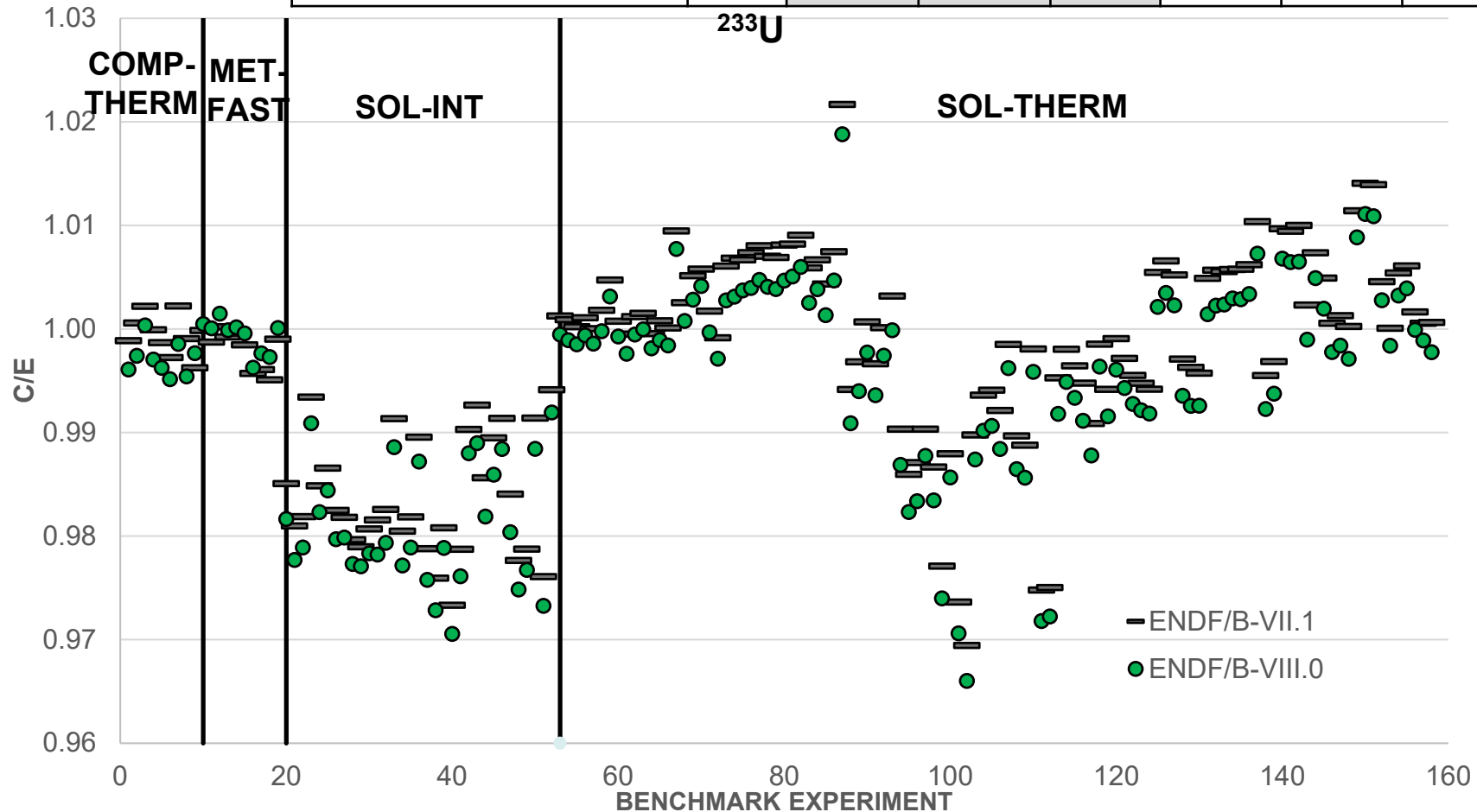| Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: MIX	73	0.70	1.0035	0.0060	0.61	1.0018	0.0058
WHISPER: IEU	13	0.43	1.0024	0.0038	0.32	1.0005	0.0033
WHISPER: LEU	209	0.28	0.9995	0.0028	0.28	0.9994	0.0027

Results of Whisper Library, 158 ^{233}U cases

- **ENDF/B-VIII.0**
  - Better UMF
  - Poor performance in intermediate & thermal energy for –VII.1 & –VIII.0

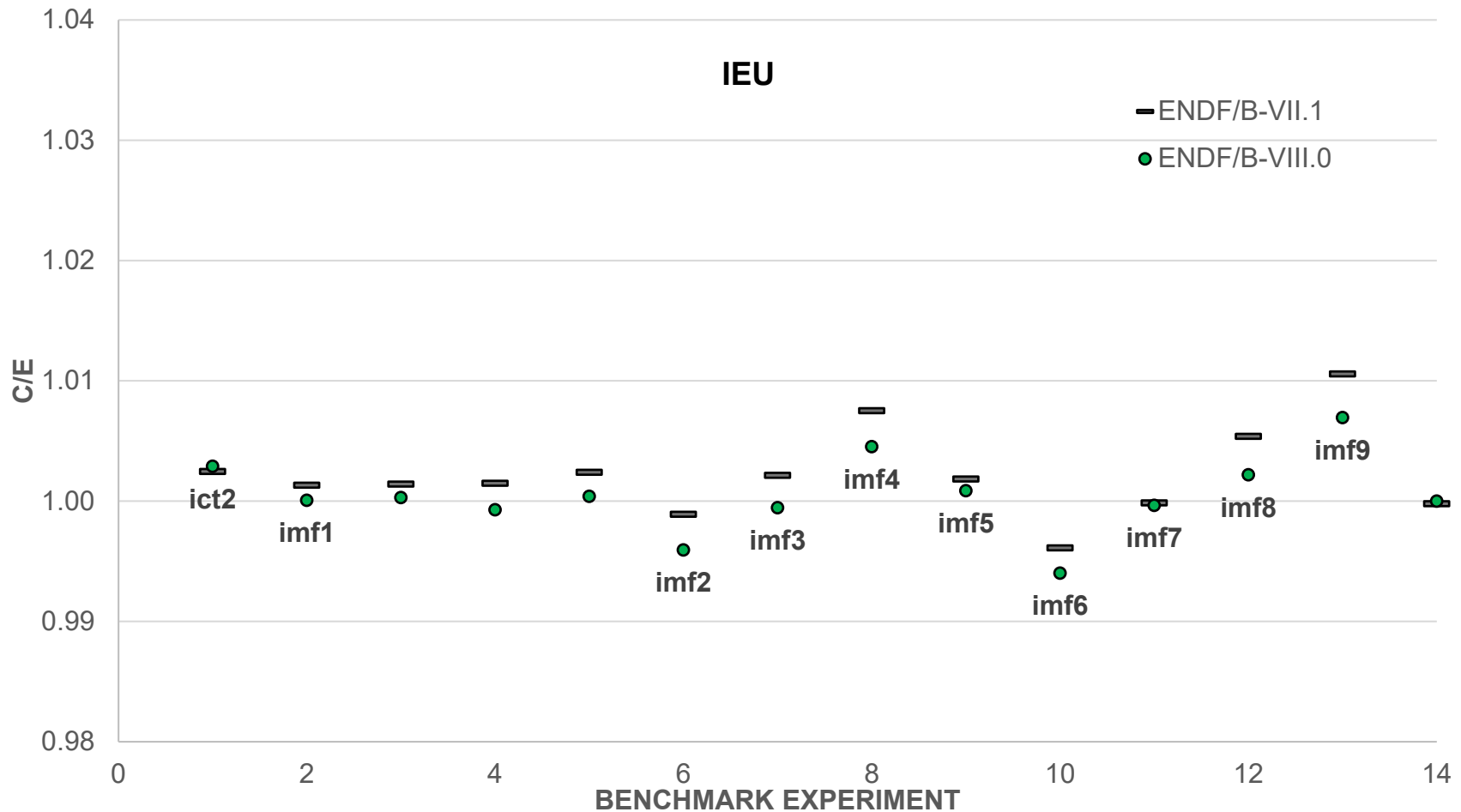| Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: ^{233}U	**158**	**1.06**	**0.9964**	**0.0100**	**1.18**	**0.9939**	**0.0102**
WHISPER: ^{233}U: COMP-THERM	9	0.20	0.9995	0.0020	0.33	0.9971	0.0016
WHISPER: ^{233}U: MET-FAST	10	0.25	0.9982	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

Extra Slides

Results of Whisper Library, 14 IEU cases

- **ENDF/B-VIII.0 results**

  – **Improved for IEU**

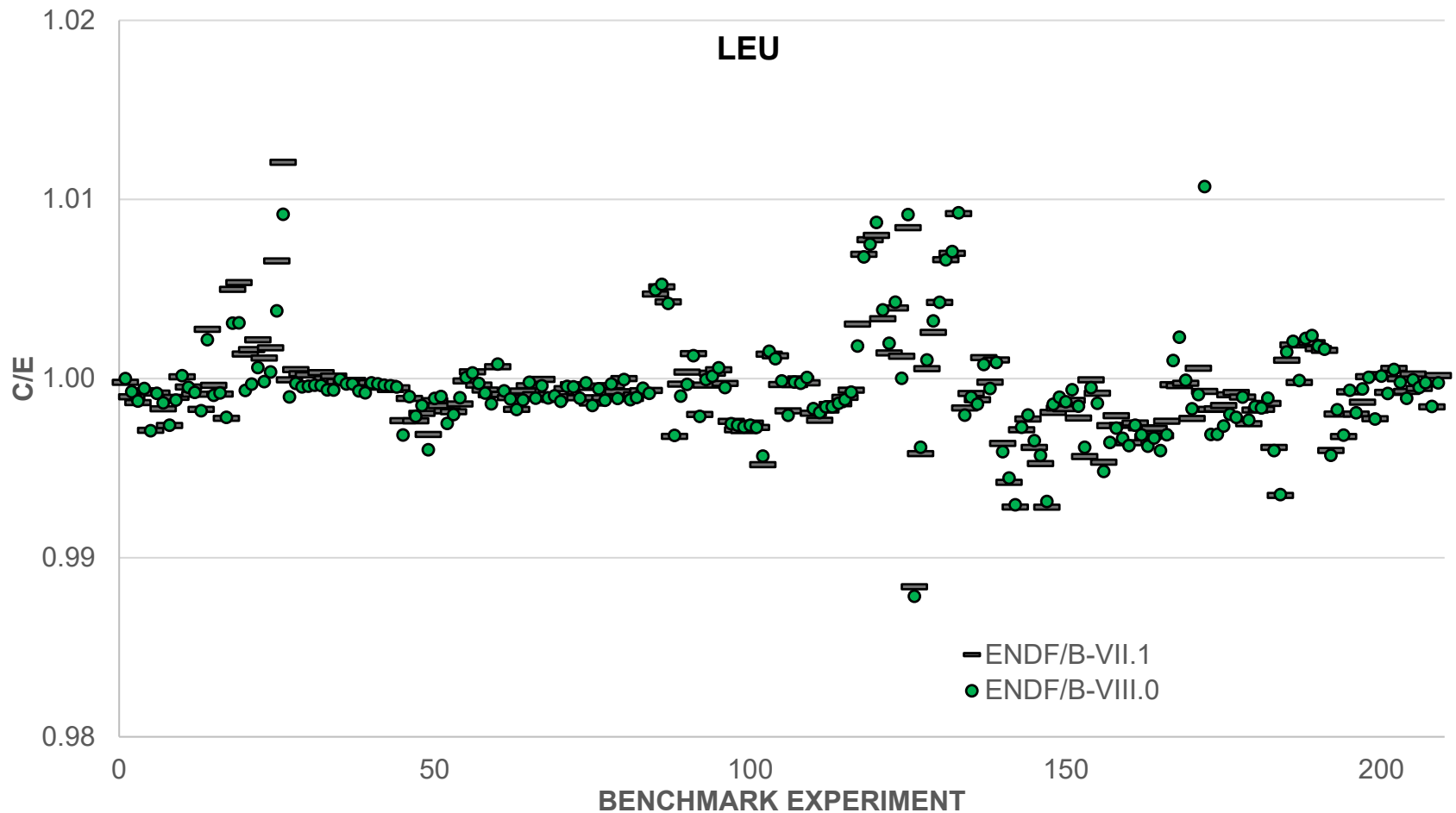| Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: IEU	13	0.43	1.0024	0.0038	0.32	1.0005	0.0033

Results of Whisper Library, 209 LEU cases

- **ENDF/B-VIII.0 results**
  - **Same for LEU**

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: LEU	**209**	**0.28**	**0.9995**	**0.0028**	**0.28**	**0.9994**	**0.0027**

Results of Whisper Library, 73 MIX cases

- **ENDF/B-VIII.0 results**

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

  – **Improved for MIX**

  – **MMF4,7 improved be-met**
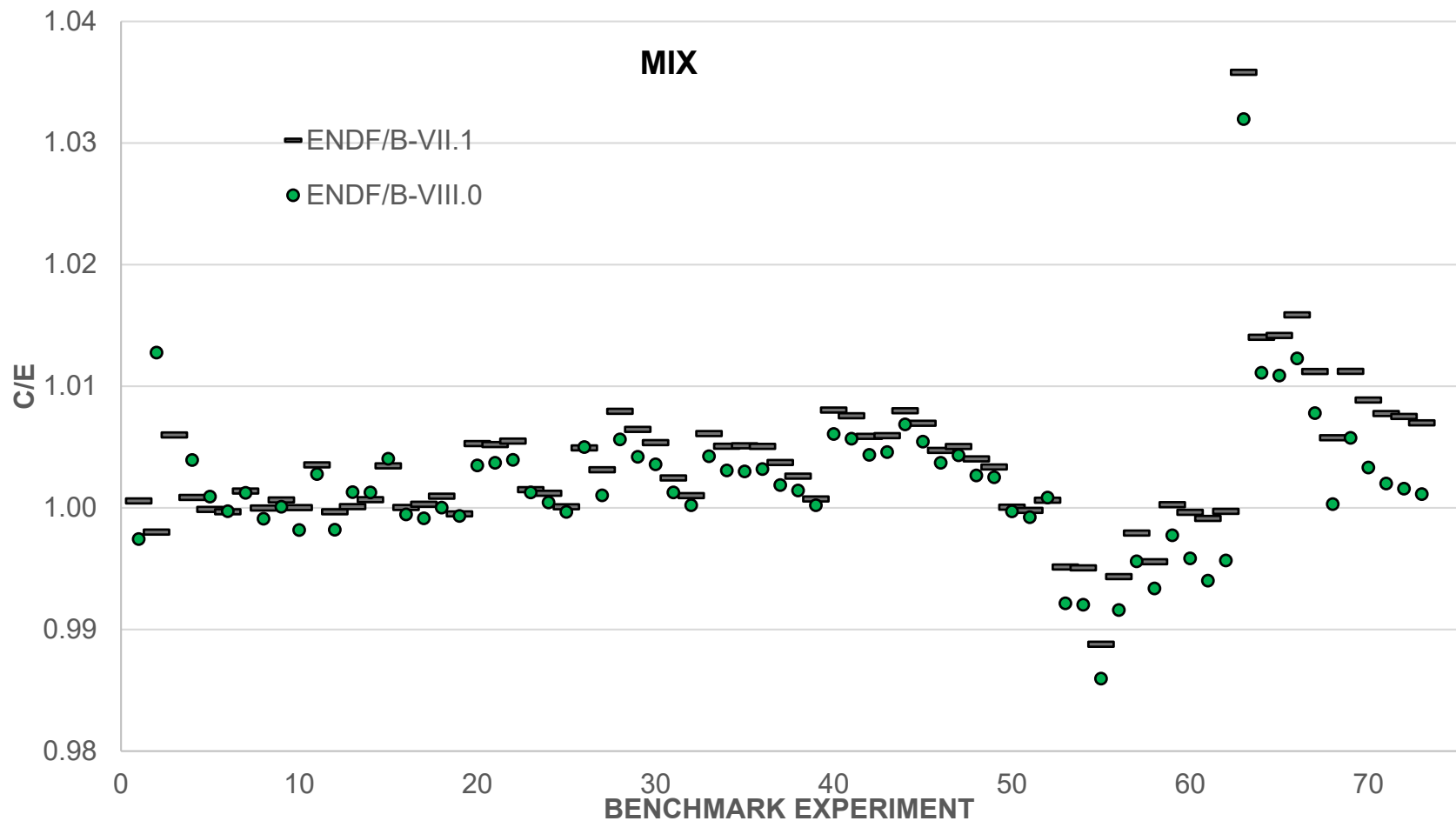
Results of Whisper Library, 19 ^{233}UCT,MF cases

- ## ENDF/B-VIII.0

- Improved UCT004 w/ d-d2o, improved UMF

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

Results of Whisper Library, 33 ^{233}USI cases

- **ENDF/B-VIII.0**

  – **Poor performance in USI for –VII.1 & 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: SOL-INTER	33	1.72	0.9837	0.0056	1.99	0.9809	0.0056

^{233}U-SOL-INTER
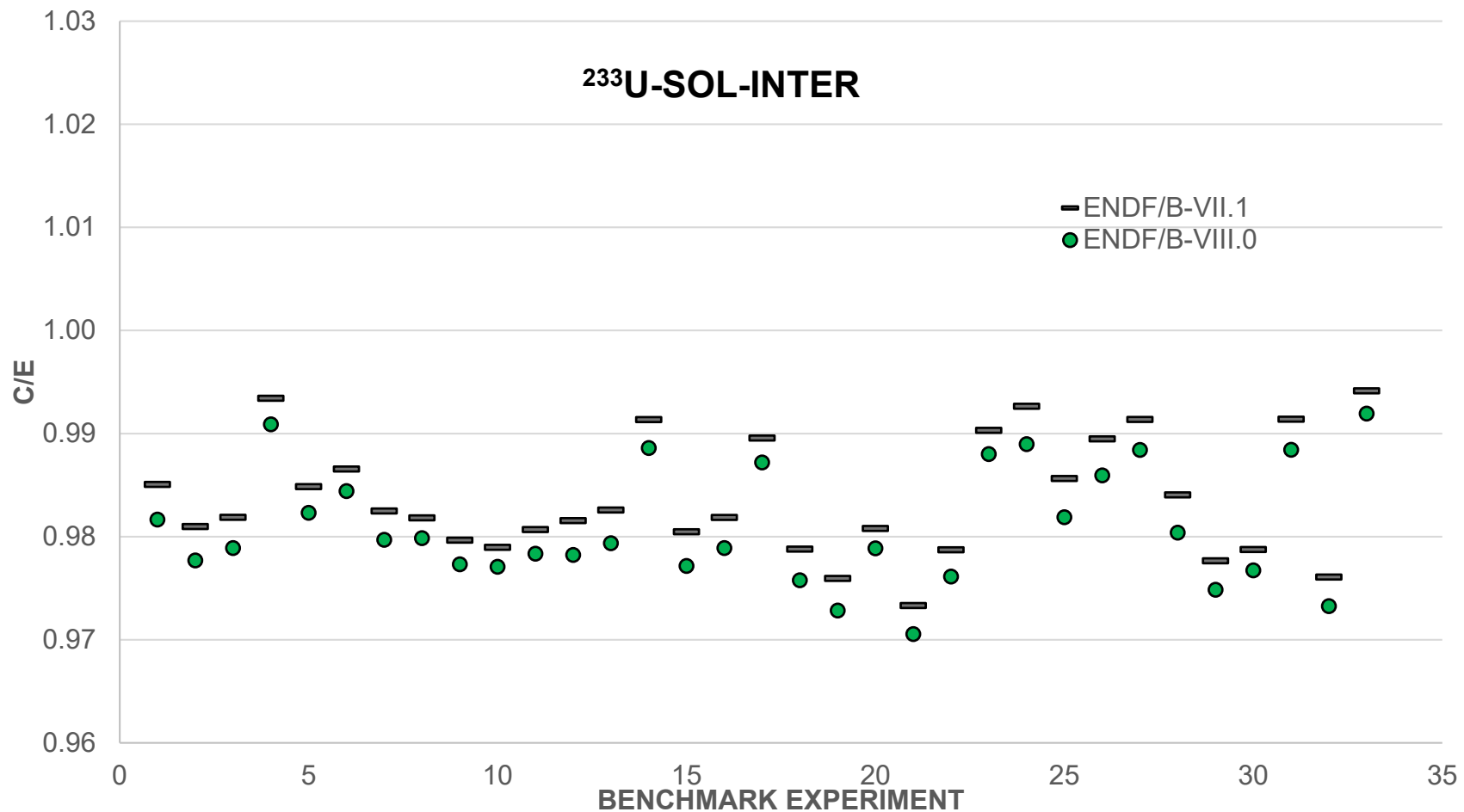
Results of Whisper Library, 106 ^{233}UST cases

- **ENDF/B-VIII.0**
  - **Poor performance in UST thermal energy for –VII.1 & 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: SOL-THERM	106	0.87	0.9999	0.0087	0.92	0.9971	0.0088

^{233}U-SOL-THERM

Thermal Scattering Library

- **S(alpha,beta) dataset names**

	ENDF/B-VII.1 →	**ENDF/B-VIII.0**
H in light water	lwtr	h-h2o
ice	--	h-ice, o-ice
D in heavy water	hwtr	d-d2o, o-d2o
polyethylene	poly	h-poly
beryllium metal	be	be-met
beryllium oxide	be-o, o-be	be-beo, o-beo
zirc-hydride	h-zr, zr-h	h-zrh, zr-zrh
lucite	--	h-luci
graphite	grph	grph (crystalline)
		grph10 (10% porous)
		grph30 (30% porous)

.... others ......