Validation of ENDF/B-VIII.1-β0-based Continuous Energy Data Tables

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XCP-5: Materials and Physical Data
Los Alamos National Laboratory

2022 CSEWG Annual Meeting – Nuclear Data Validation

LA-UR-22-31596

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Introduction

- Nuclear data library ENDF/B-VIII.1-β0 files released early October 2022
- Changes from ENDF/B-VIII.0 →

```
– 28,29,30Si taken from INDEN: ORNL/LTR-2018/1044 (M. Pigni et al., 2018)
– 50,53,54Cr taken from INDEN: v2.3.2, NDS 173, 1-41 (2021)
– 52Cr taken from INDEN: v2.3.4 (cr52v234c), NDS 173, 1-41 (2021) + RRR changes
– 54Fe taken from INDEN: fe54e80p
– 56Fe taken from INDEN: fe56e80X29r50
– 57Fe taken from INDEN: fe57e80o
– 63Cu taken from INDEN: cu63ane6k09aRR
– 65Cu taken from INDEN: cu65ane5k05
– 233U taken from INDEN: u233ornl_2b_nu12
– 235U taken from INDEN: u235ib46o28t6DNcnu5ef0ST25d
– 238U taken from INDEN (with Q-value fix): u238e80u8V02b + GitLab commit ff23a85b
```

- Designation of *a*, *b*, or *c* based on Pu-239 Evaluation:
  - (a) INDEN file (β0a.1) *pu239p57*
  - (b) LANL file from 05/25/2022 (β0b.1) *lanl_05l25l2022_n_94-Pu-239.endf*
  - (c) LLNL file (β0c.1) *yi01za094239.endl2022-ex4+0.17pc*
- This analysis also includes an updated LANL evaluation from 10/17/2022 (β0b.2) *lanl_10l17l2022_n_94-Pu-239.endf*

- Continuous-energy tables were processed with NJOY2016 into ACE (a continuous energy) formatted files
- Validation was performed using ICSBEP benchmarks [1] with the MCNP® code, version 6.2 [2]

Background

- **Neutron Reactor Kinetics Parameters:**

(1) Prompt neutron decay constant (α) – measures time rate of change of the prompt neutron population

$$\alpha = \frac{k_p - 1}{l}$$

k_p: prompt neutron multiplication factor, l: mean neutron lifetime

(2) Effective Delayed Neutron Fraction (β_{eff}) – measures effectiveness of the delayed neutron population causing fission

$$\beta_{\text{eff}} = 1 - \frac{k_p}{k}$$

- **Validation Metrics:**
- Bias = Calculated Value (C) – Experimental Value (E)
- Mean Absolute Bias (“Mean Abs. Bias” in figures) = $\frac{|C-E|}{n}$

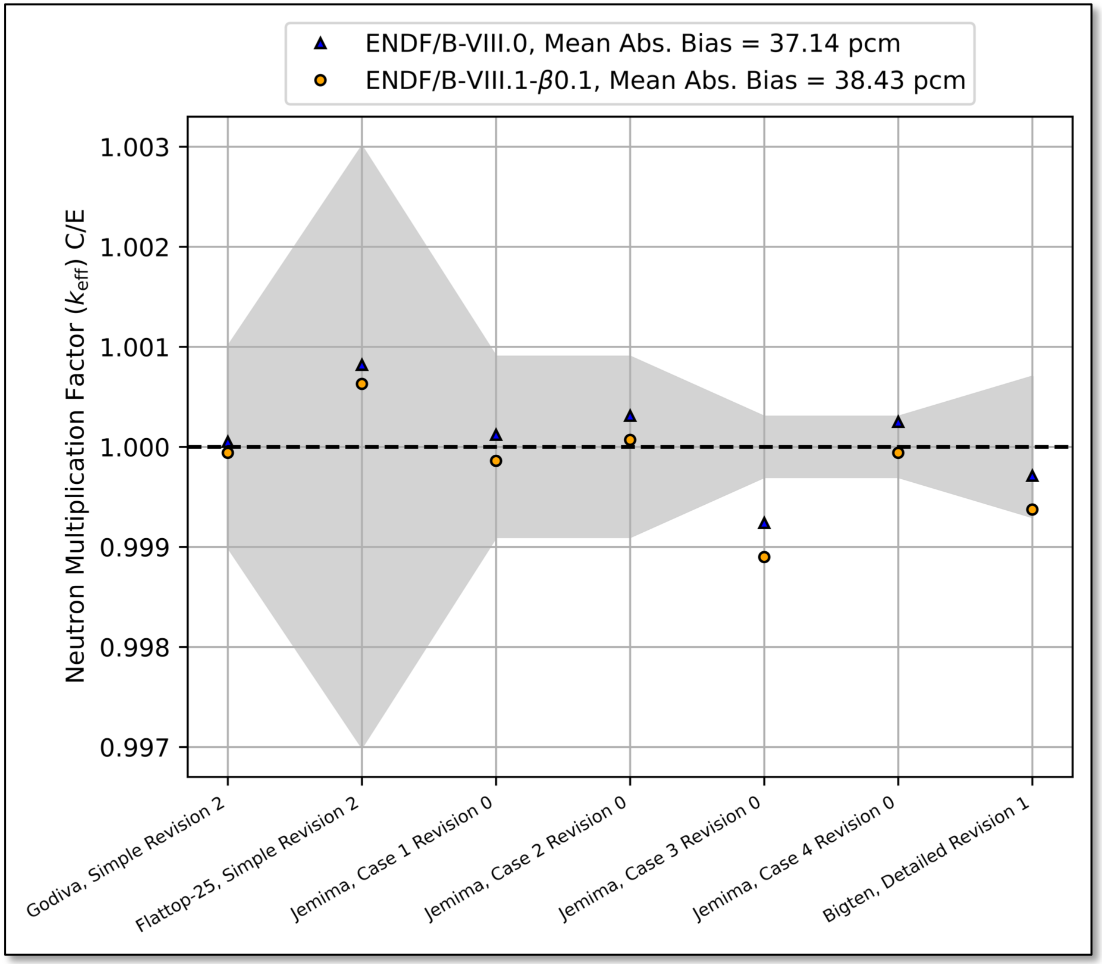
n: number of benchmark experiments

- **Relative Sensitivity Coefficient Calculation:**

σ: some nuclear data

$$S_{k_{\text{eff}},\sigma} = \frac{\sigma}{k_{\text{eff}}} \frac{\partial k_{\text{eff}}}{\partial \sigma}$$

Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides, Non-Pu Legacy Benchmark Suite



	Bias (pcm)	
Benchmark	ENDF/B-VIII.0	ENDF/B-VIII.1-β0.1
Godiva	**+5**	-6
Flattop-25	+82	**+63**
Jemima Case 1	**+12**	-14
Jemima Case 2	+31	**+7**
Jemima Case 3	**-76**	-110
Jemima Case 4	+25	**-6**
Bigten	**-29**	-63

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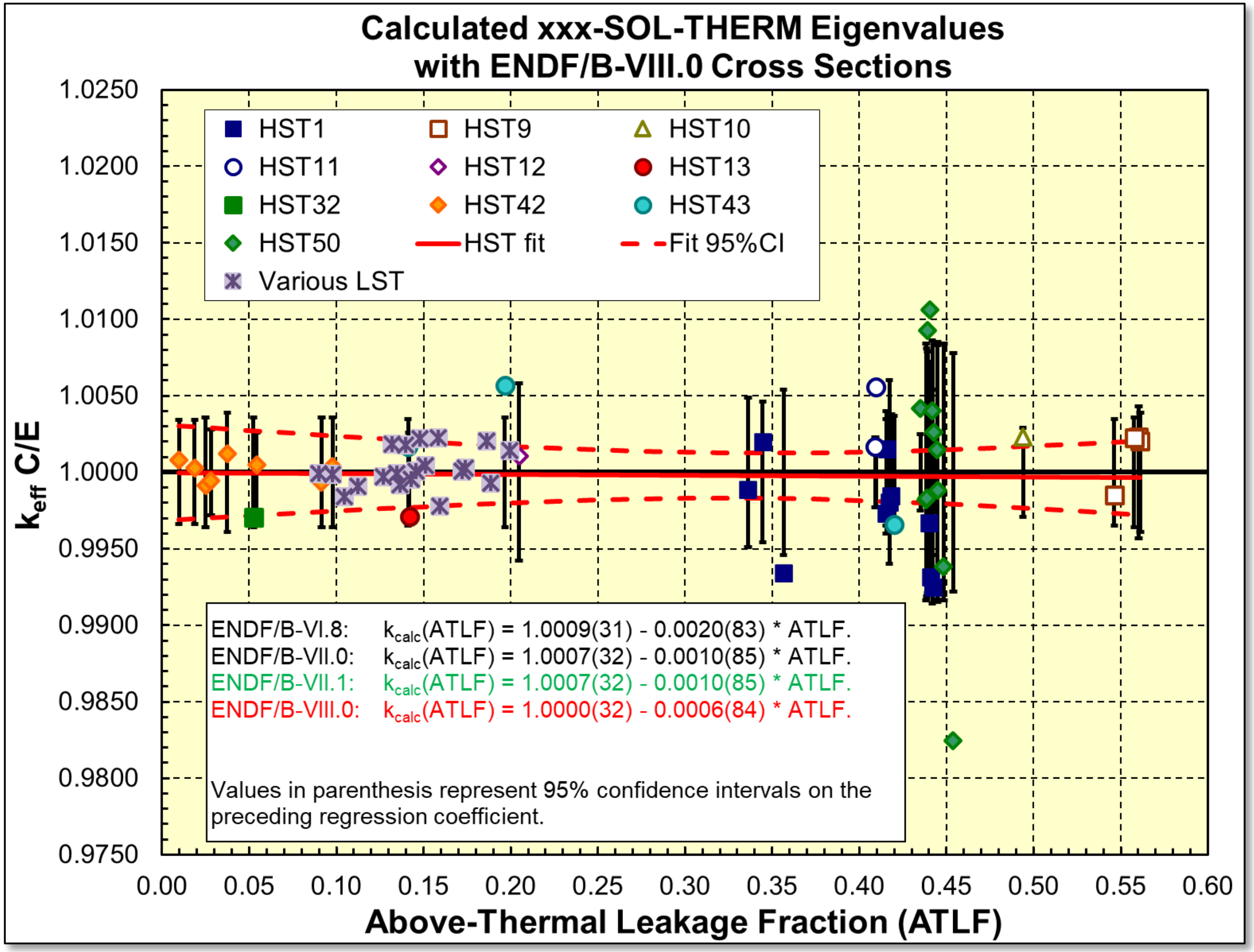
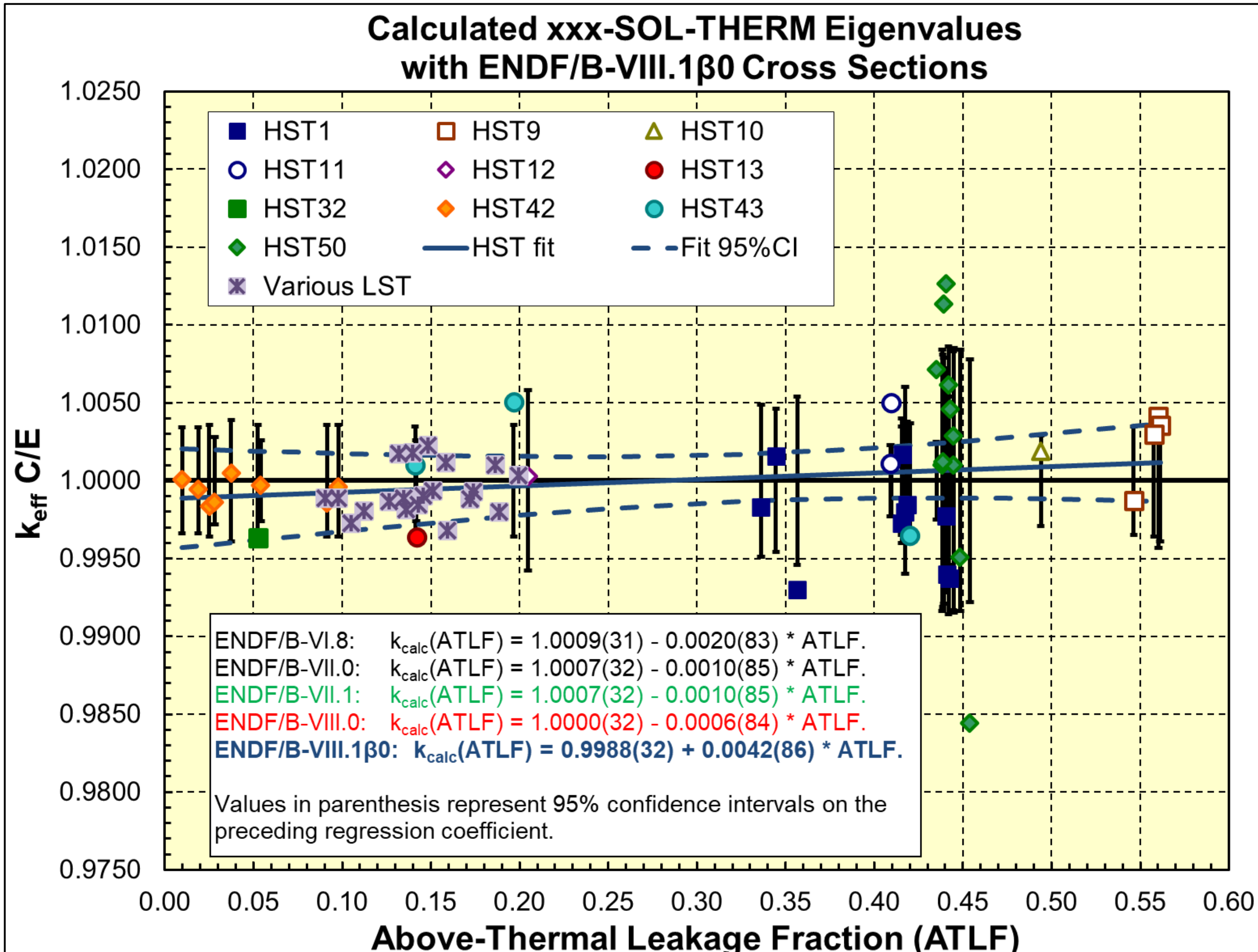
Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides



HST-01: Uranyl Nitrate
HST-09: Uranium Oxyfluoride
HST-10: Uranium Oxyfluoride
HST-11: Uranium Oxyfluoride
HST-12: Uranium Oxyfluoride
HST-13: Uranium Nitrate
HST-32: Uranyl Nitrate
HST-42: Uranium Nitrate
HST-43: Uranium Oxyfluoride
HST-50: Uranyl Fluoride

Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides



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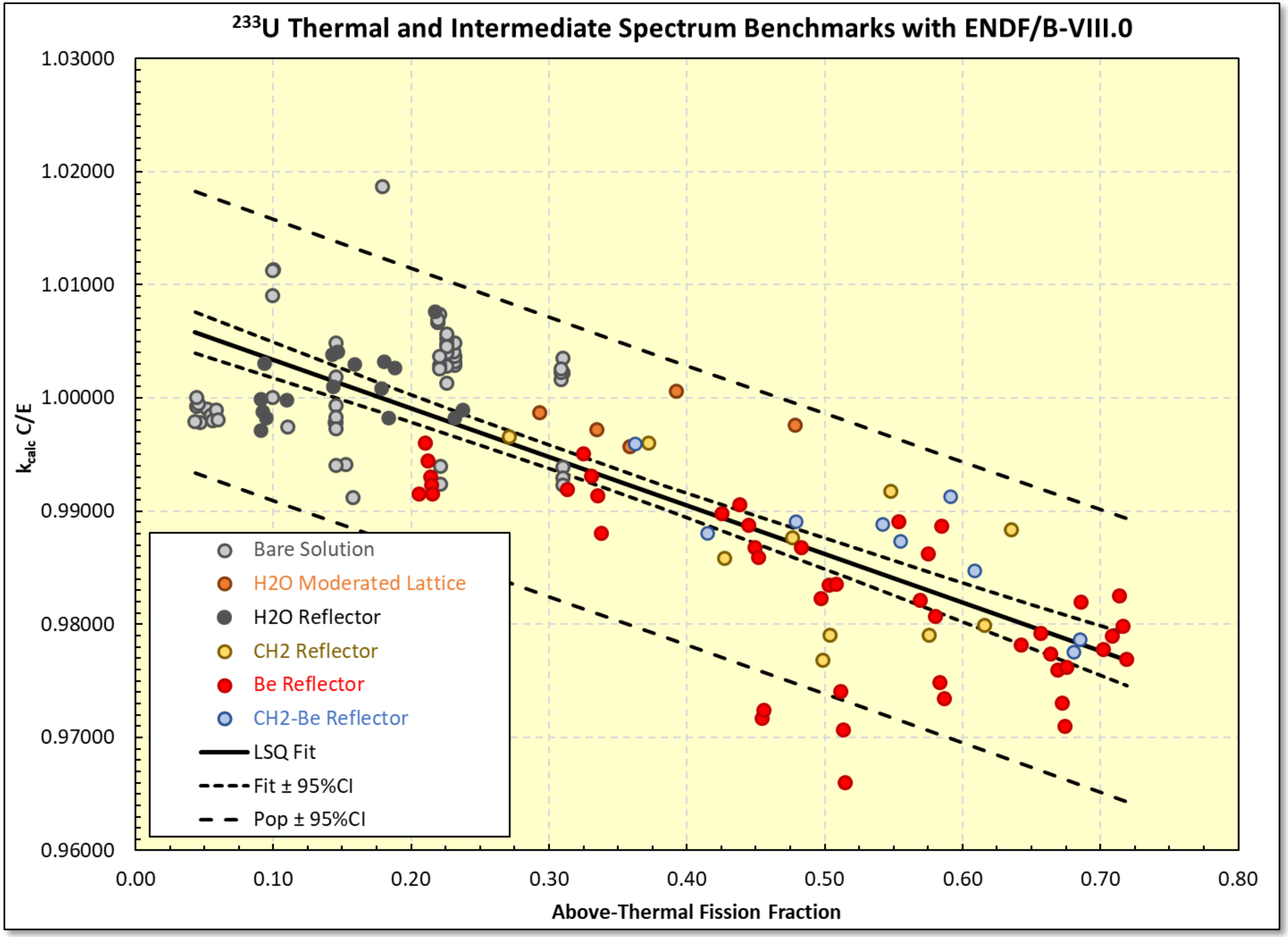
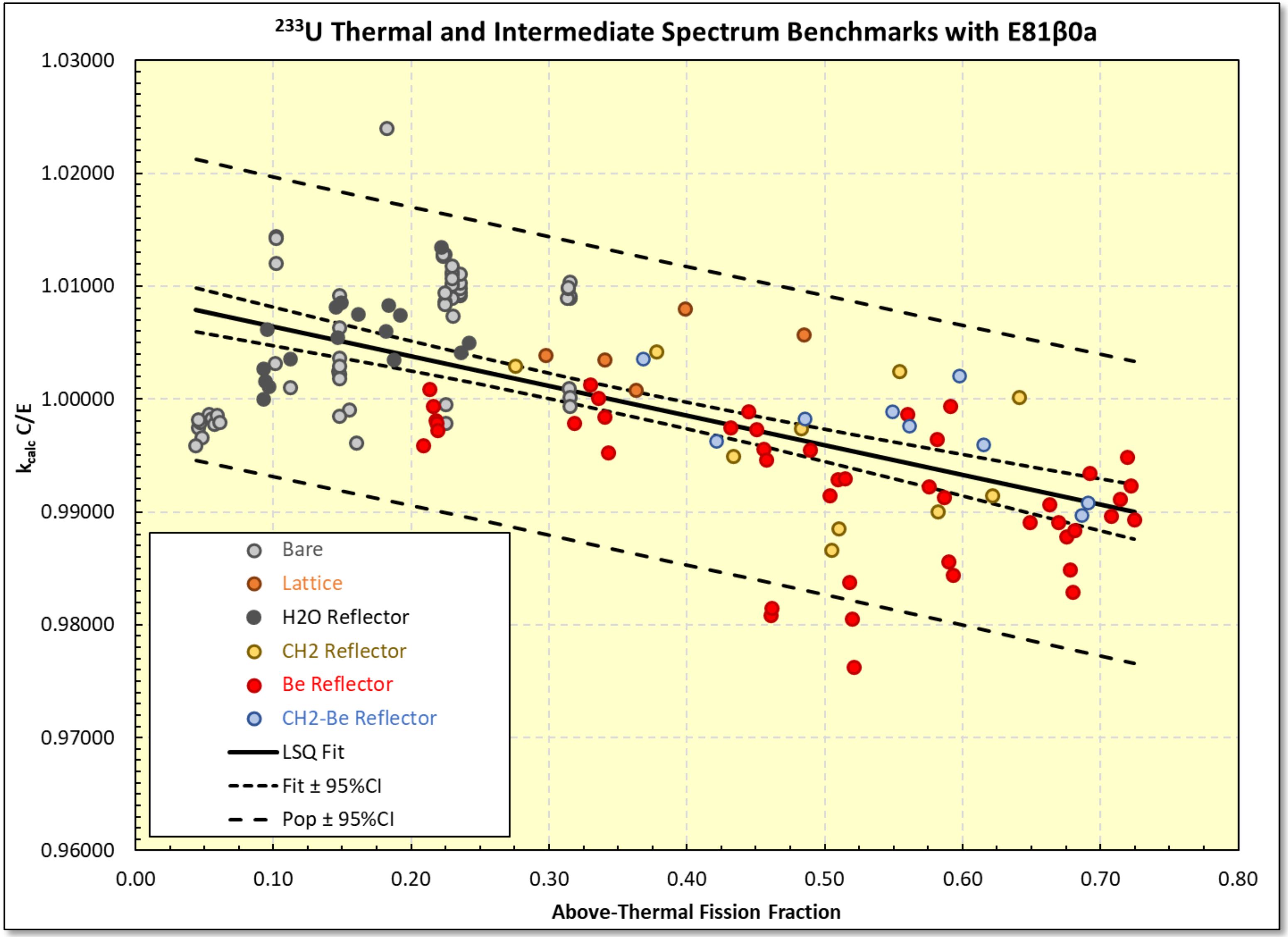
HST-13: Uranium Nitrate
HST-32: Uranyl Nitrate
HST-42: Uranium Nitrate
HST-43: Uranium Oxyfluoride
HST-50: Uranyl Fluoride

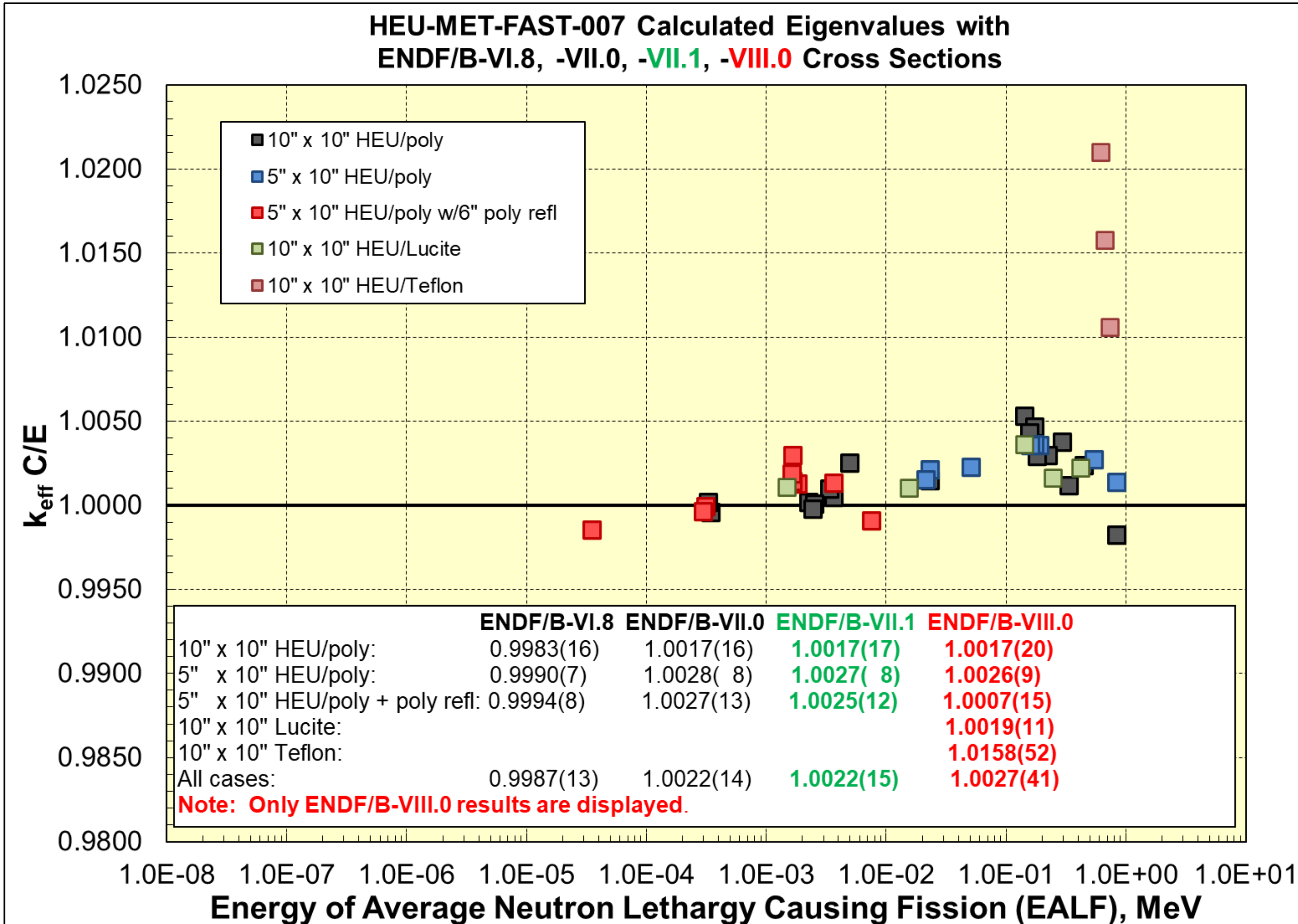
Results – ENDF/B-VIII.0 S(α, β), ENDF/B-VIII-β0 nuclides



Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides



Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides



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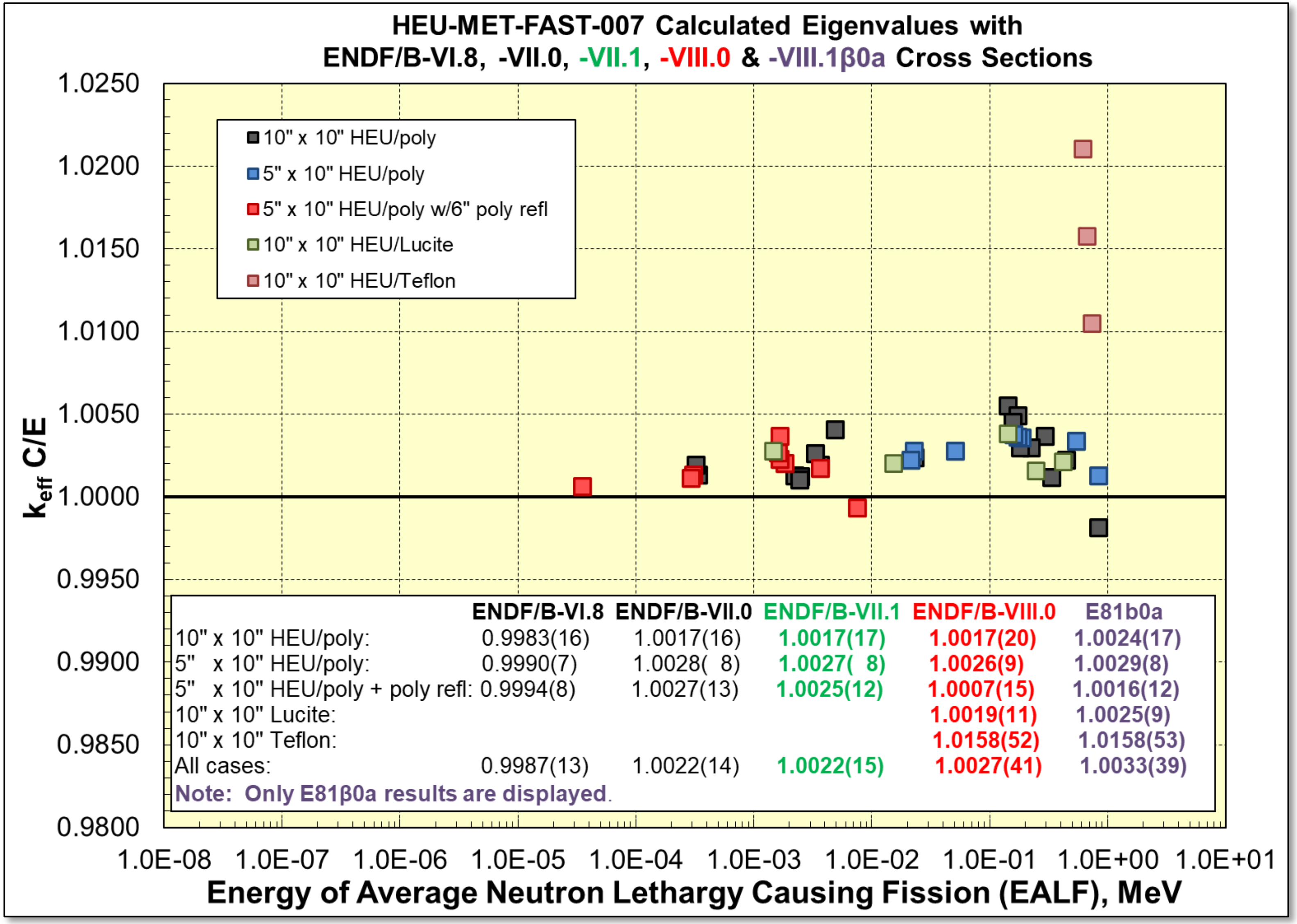
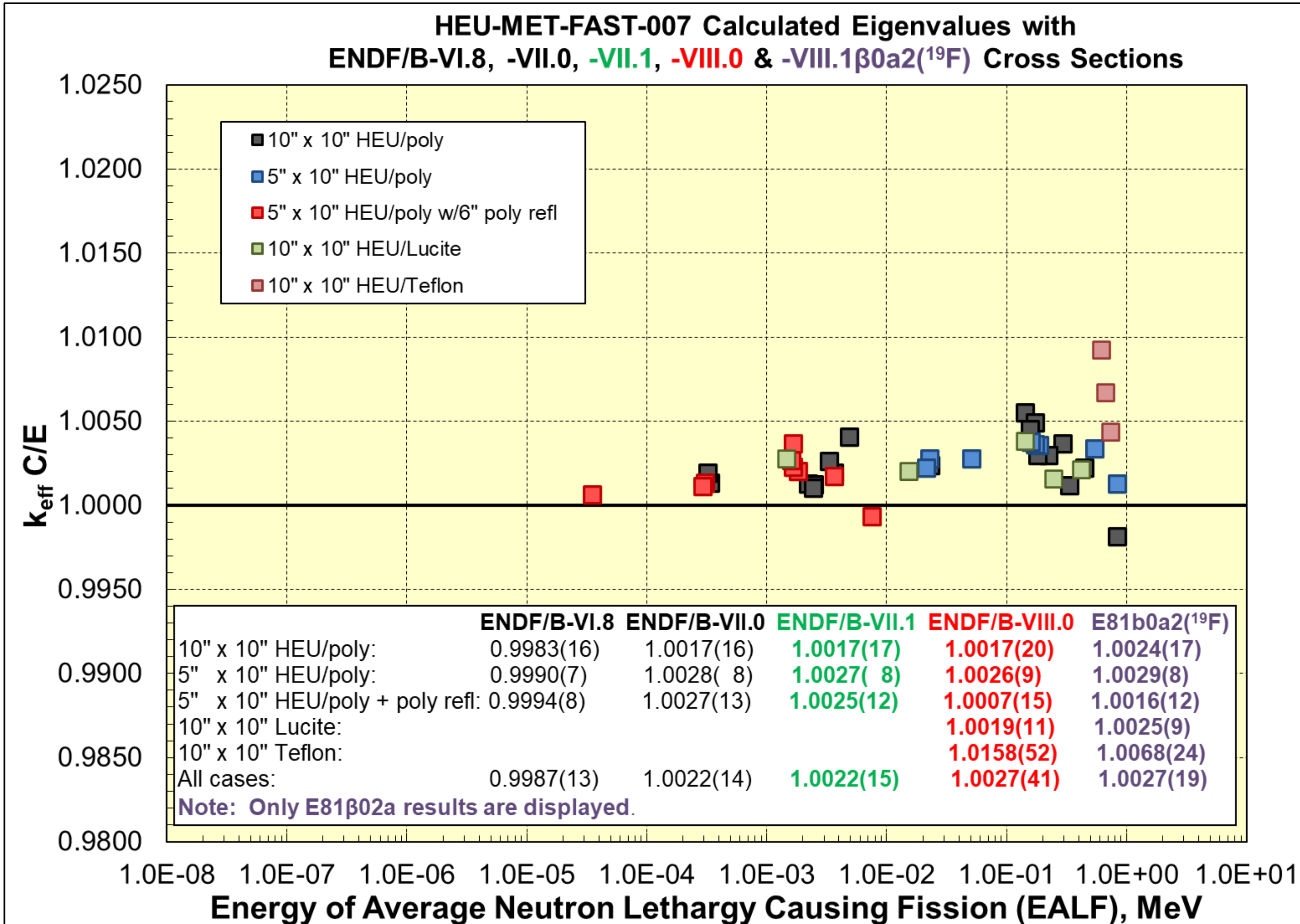
Results – ENDF/B-VIII.0 S(α, β), ENDF/B-VIII-β0 nuclides



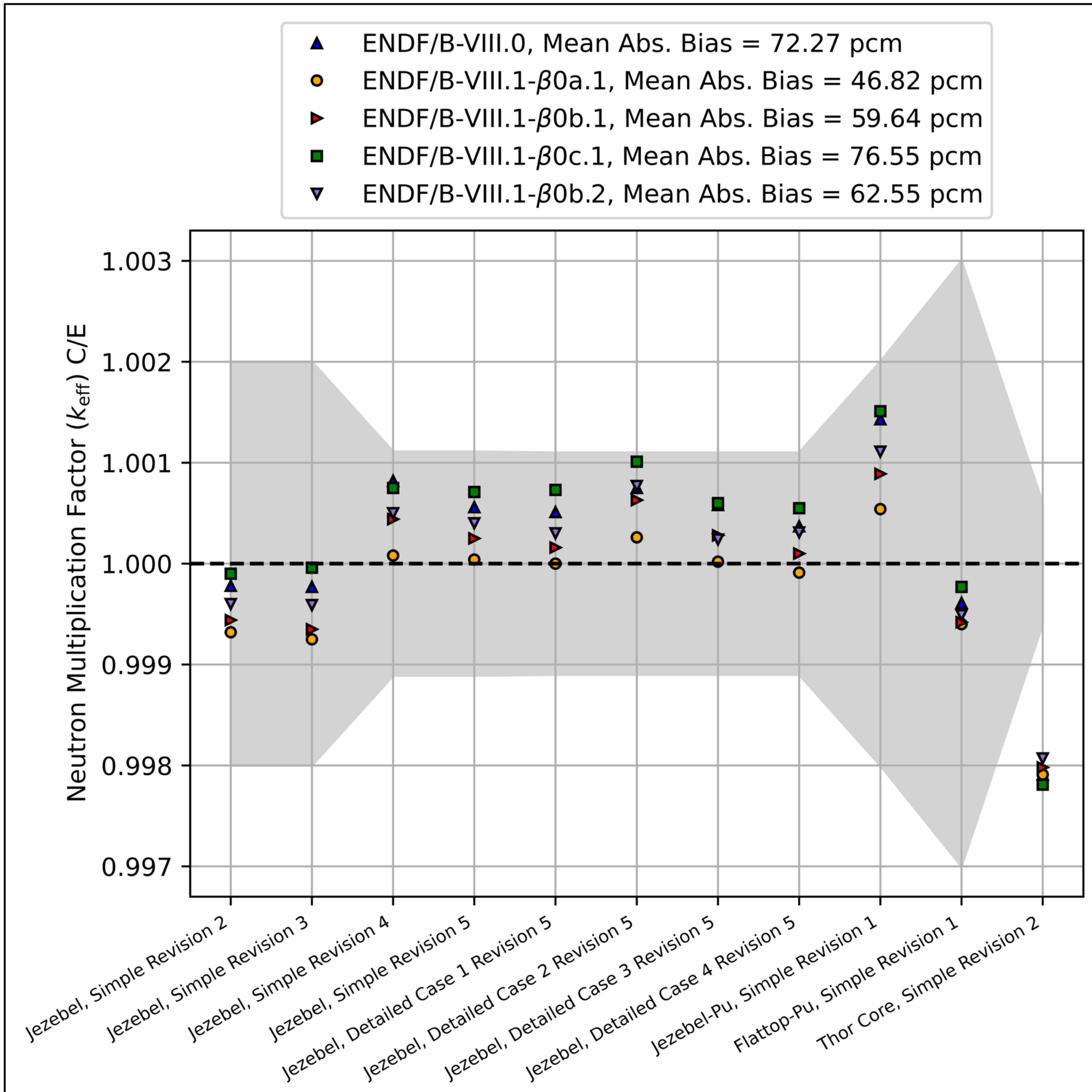
Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides



	ENDF/B-VI.8	ENDF/B-VII.0	ENDF/B-VII.1	ENDF/B-VIII.0	E81b0a2(19F)
10" x 10" HEU/poly:	0.9983(16)	1.0017(16)	1.0017(17)	1.0017(20)	1.0024(17)
5" x 10" HEU/poly:	0.9990(7)	1.0028(8)	1.0027(8)	1.0026(9)	1.0029(8)
5" x 10" HEU/poly + poly refl:	0.9994(8)	1.0027(13)	1.0025(12)	1.0007(15)	1.0016(12)
10" x 10" Lucite:				1.0019(11)	1.0025(9)
10" x 10" Teflon:				1.0158(52)	1.0068(24)
All cases:	0.9987(13)	1.0022(14)	1.0022(15)	1.0027(41)	1.0027(19)

Note: Only E81β02a results are displayed.

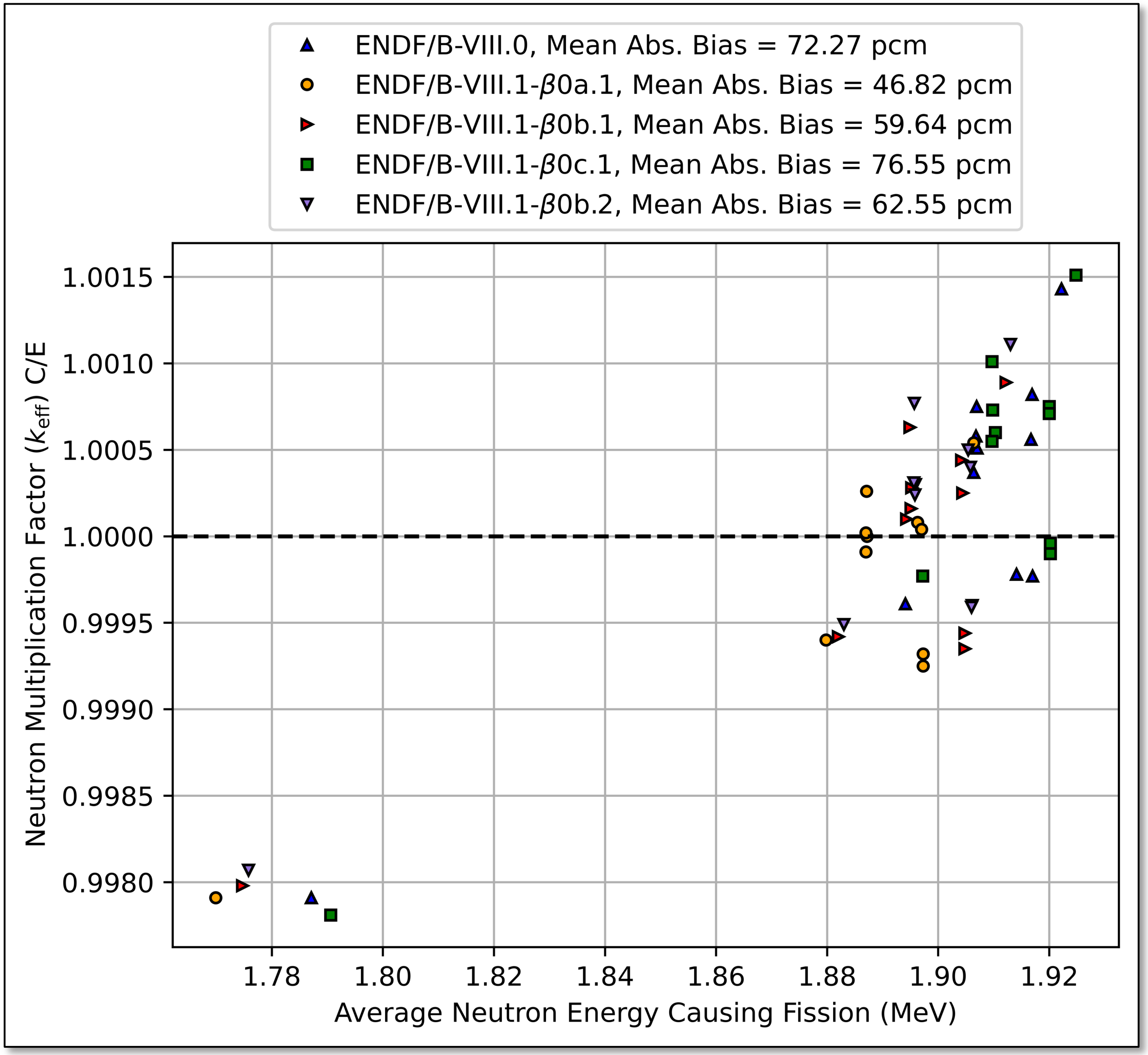
Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides, Pu Legacy Benchmark Suite



Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides, Pu Legacy Benchmark Suite

	Bias (pcm)				
Benchmark	ENDF/B-VIII.0	ENDF/B-VIII.1-β0a.1	ENDF/B-VIII.1-β0b.1	ENDF/B-VIII.1-β0c.1	ENDF/B-VIII.1-β0b.2
Jezebel Simple rev2	-22	-68	-56	**-10**	-40
Jezebel Simple rev3	-23	-75	-65	**-4**	-41
Jezebel Simple rev4	+82	**+8**	+44	+75	+50
Jezebel Simple rev5	+56	**+4**	+25	+71	+40
Jezebel Detailed rev5 Case 1	+51	**0**	+16	+73	+30
Jezebel Detailed rev5 Case 2	+75	**+26**	+63	+101	+77
Jezebel Detailed rev5 Case 3	+58	**+2**	+28	+60	+24
Jezebel Detailed rev5 Case 4	+37	**-9**	+10	+55	+31
Jezebel-Pu ("Dirty Jezebel")	+143	**+54**	+89	+151	+111
Flattop-Pu	-39	-60	-58	**-23**	-51
Thor Core	-209	-209	-202	-219	**-193**

Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides, Pu Legacy Benchmark Suite



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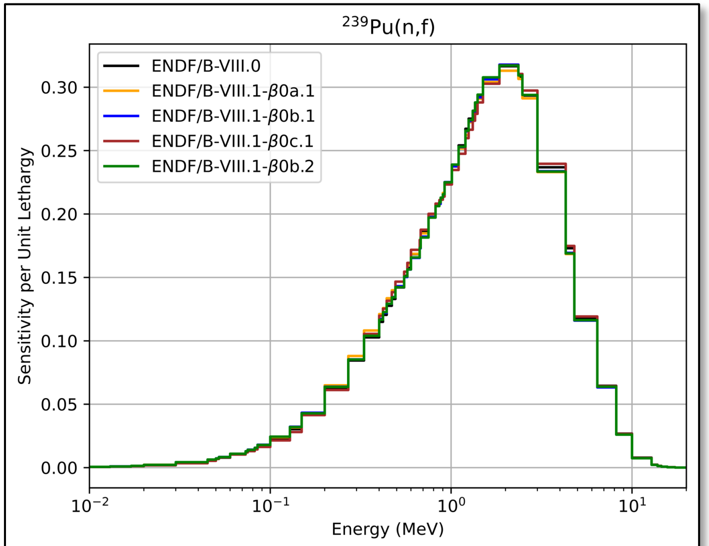
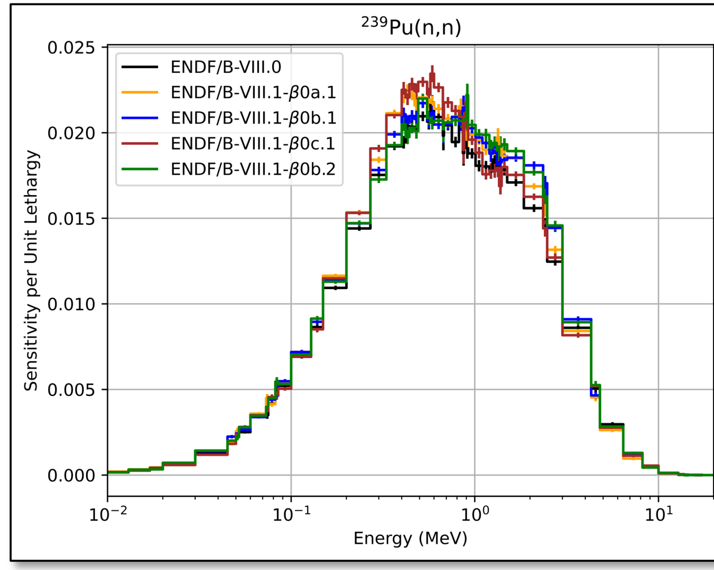
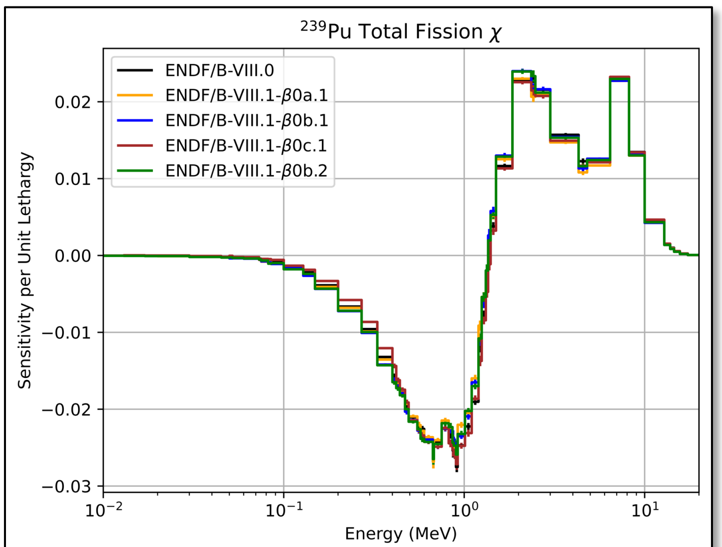
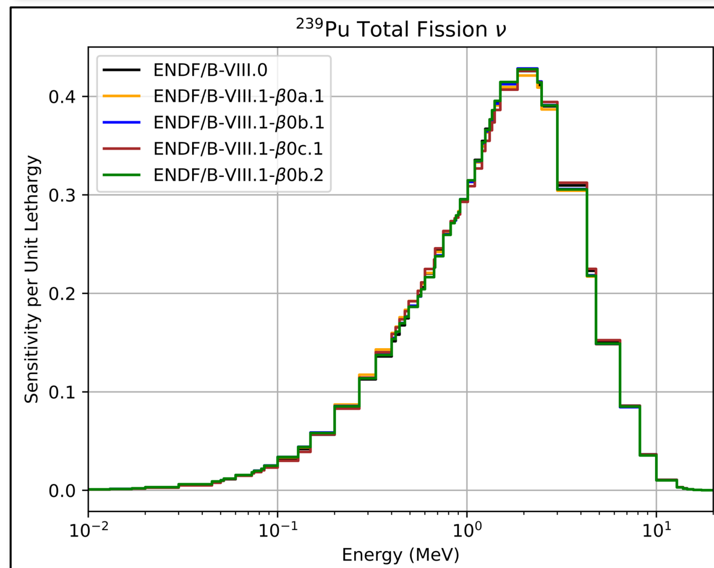
Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides, Jezebel Simple rev5 Benchmark ^{239}Pu Sensitivity

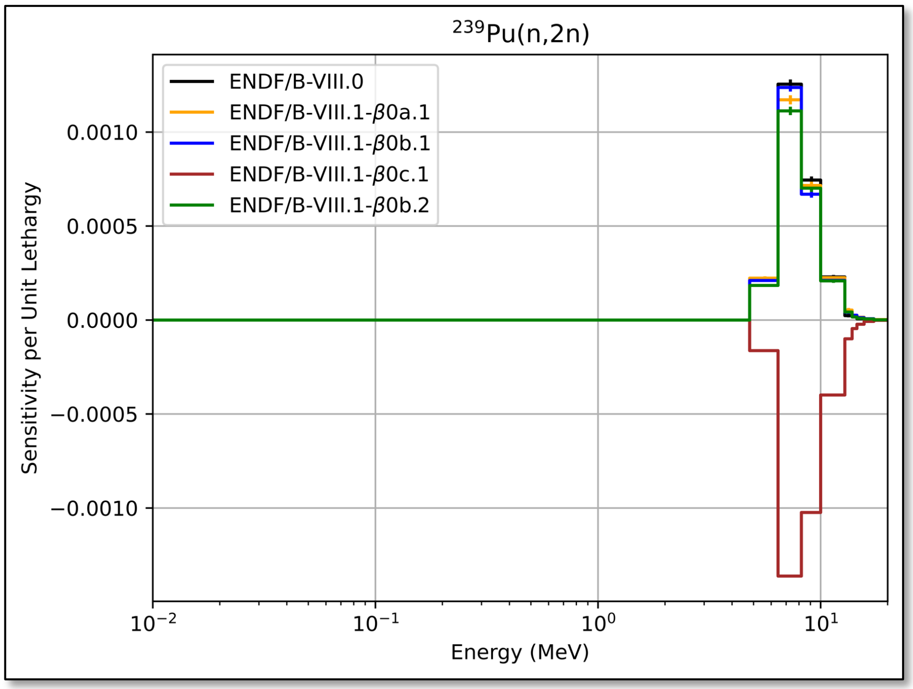


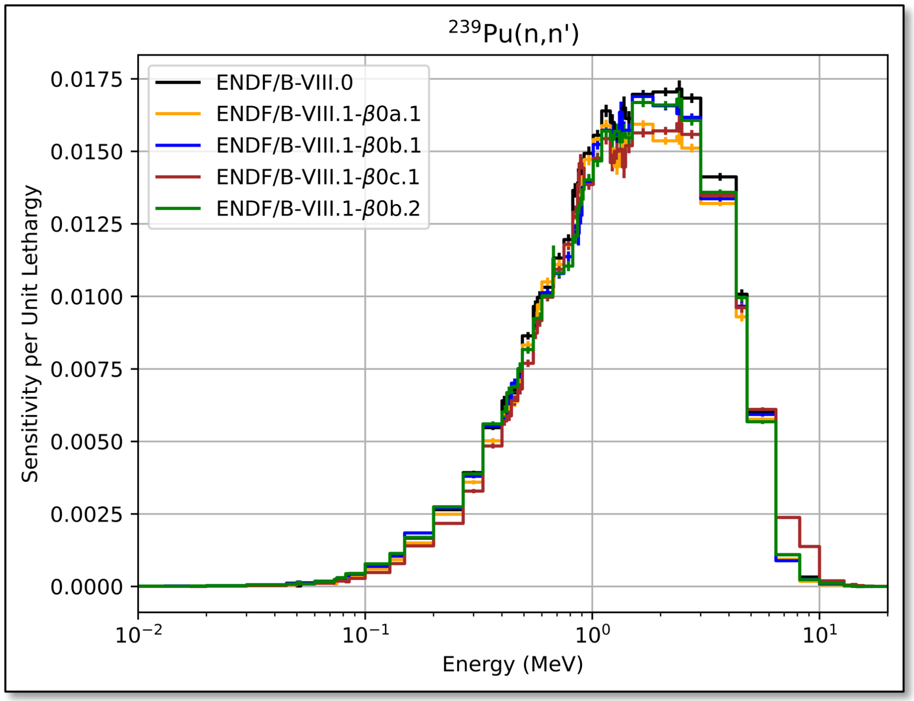






Results – ENDF/B-VIII.0 S(α, β), ENDF/B-VIII-β0 nuclides, Jezebel Simple rev5 Benchmark ^{239}Pu Sensitivity





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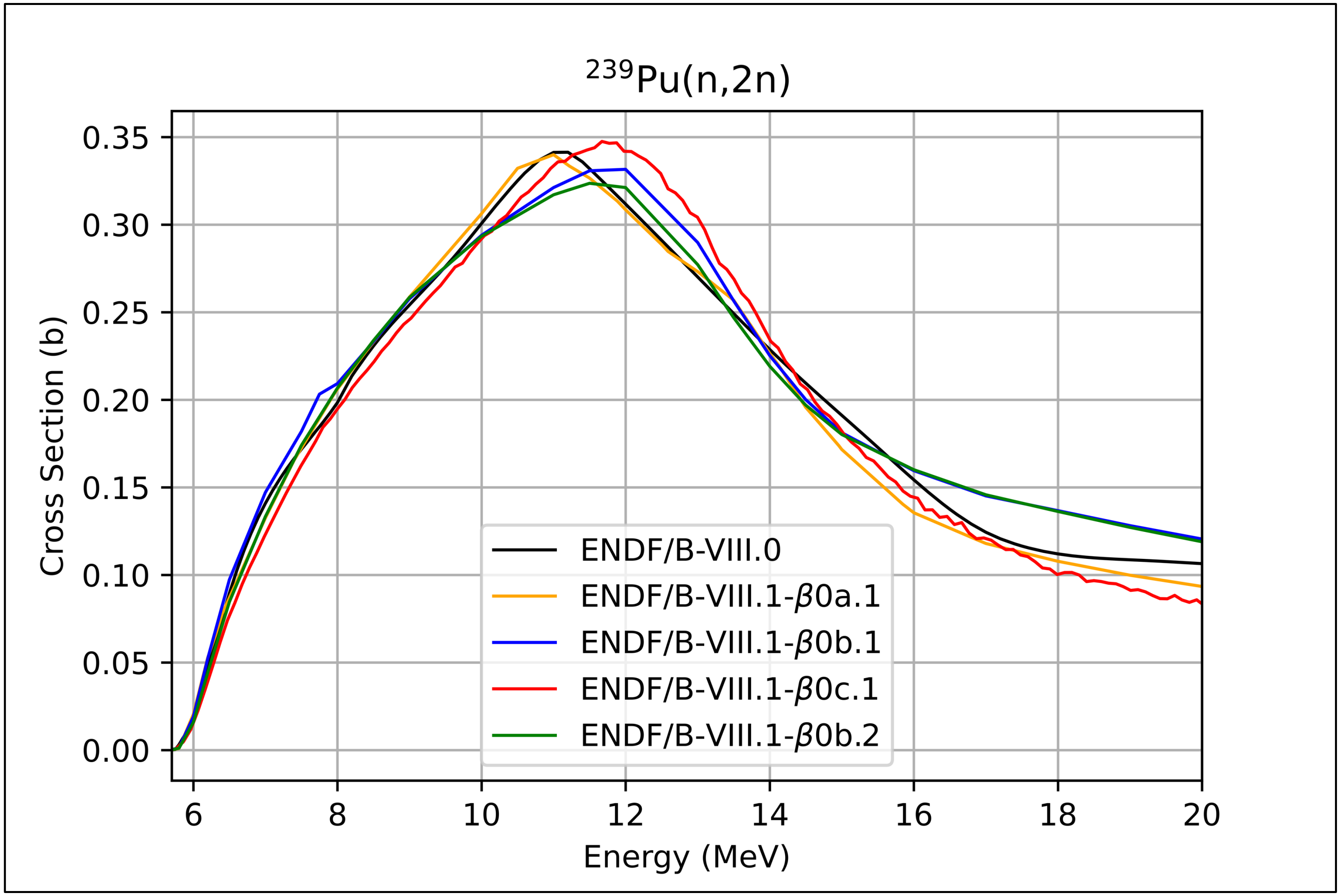
Results – ENDF/B-VIII.0 S(α, β), ENDF/B-VIII-β0 nuclides



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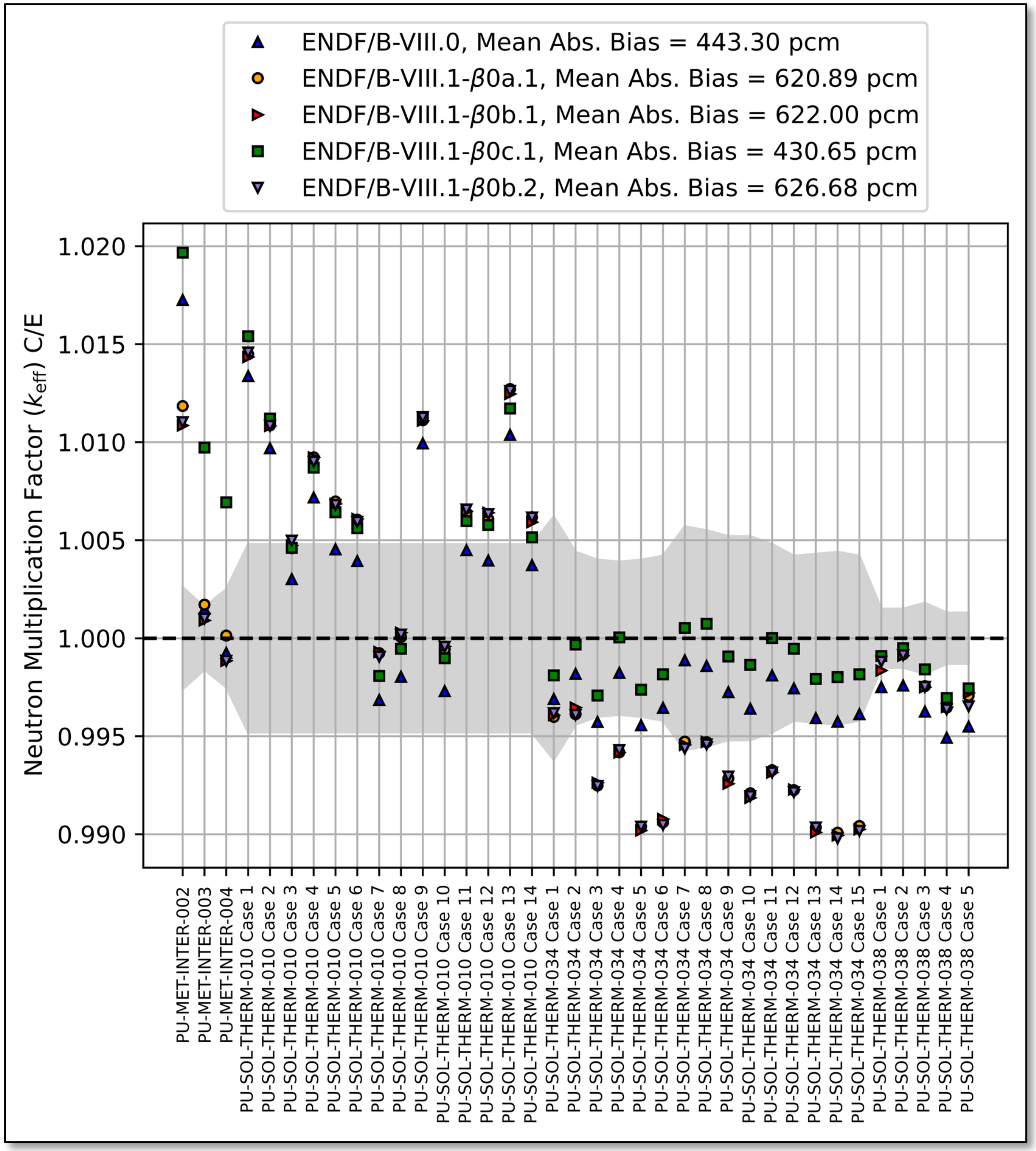
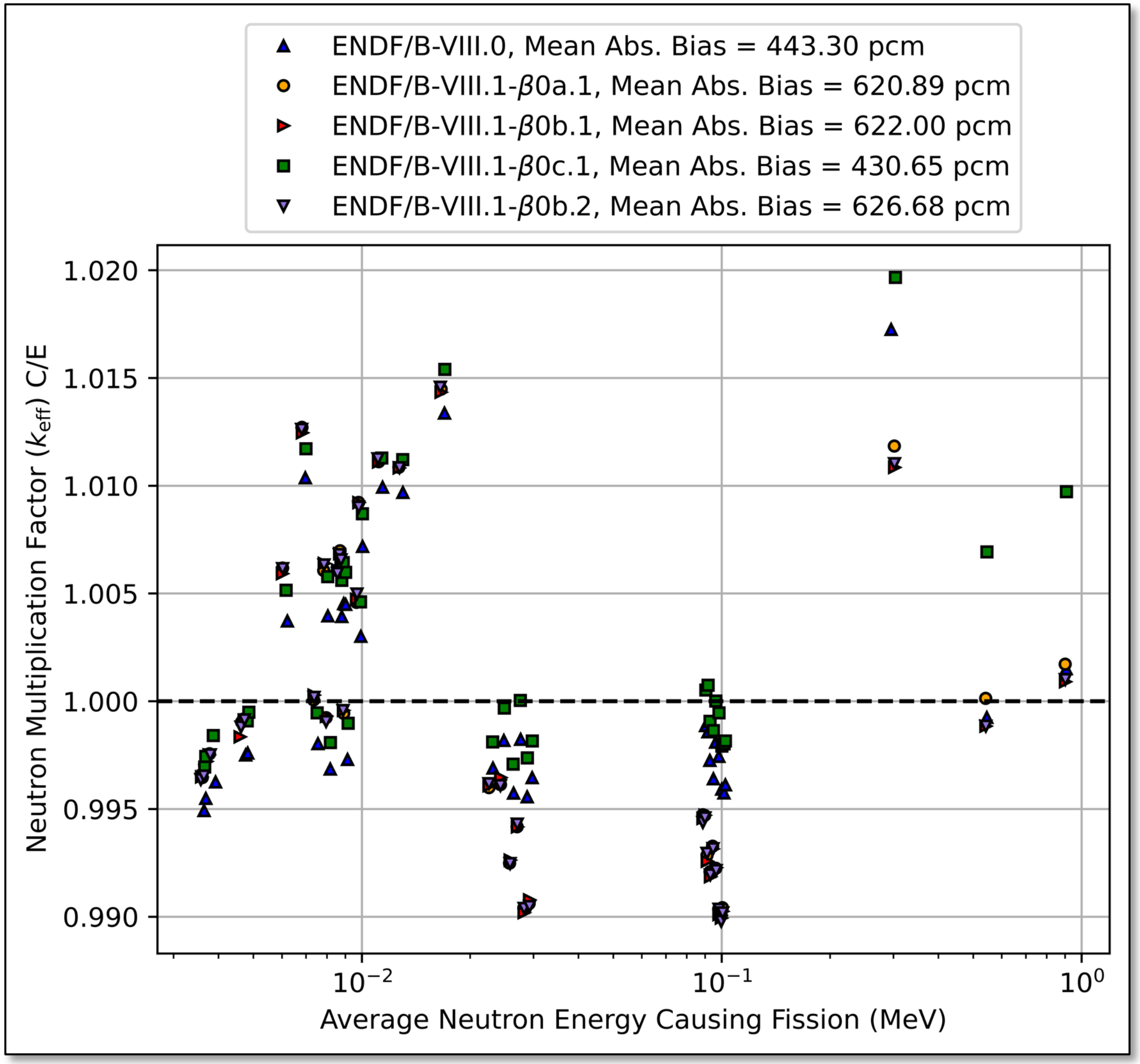
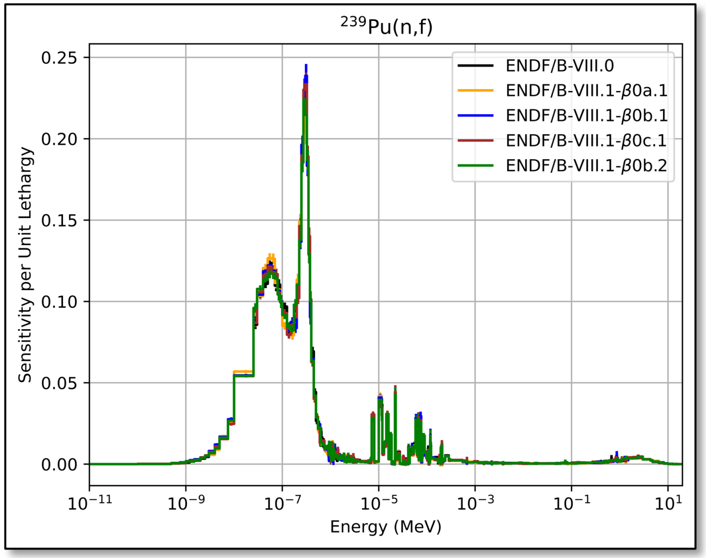
Results – ENDF/B-VIII.0 $S(\alpha,\beta)$, ENDF/B-VIII-β0 nuclides, PU-MET-INTER/PU-SOL-THERM Benchmark Suite

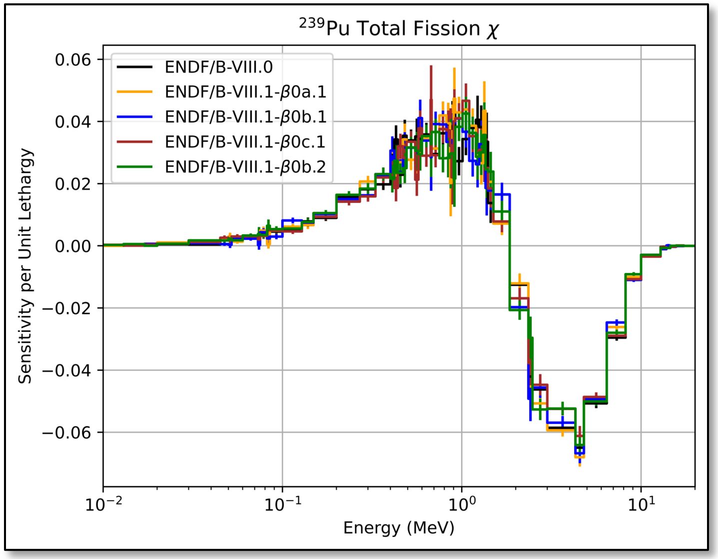


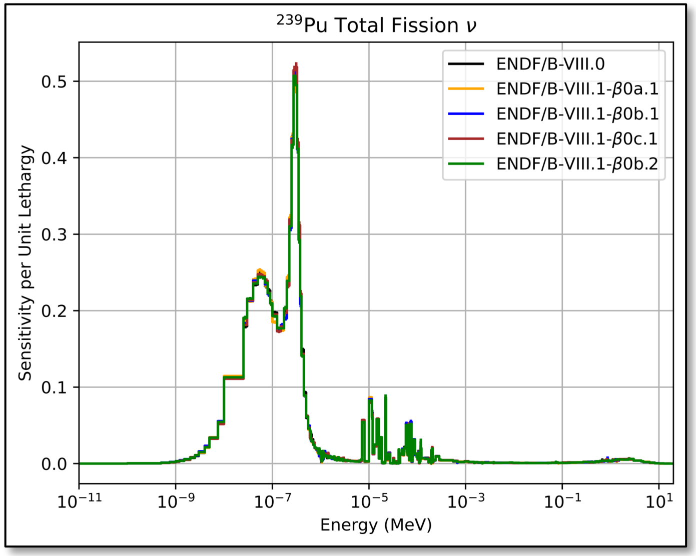
Results – ENDF/B-VIII.0 S(α, β), ENDF/B-VIII-β0 nuclides, PU-MET-INTER/PU-SOL-THERM Benchmark Suite



Results – ENDF/B-VIII.0 S(α, β), ENDF/B-VIII-β0 nuclides, PU-SOL-THERM-034 Case 2 Benchmark ^{239}Pu Sensitivity







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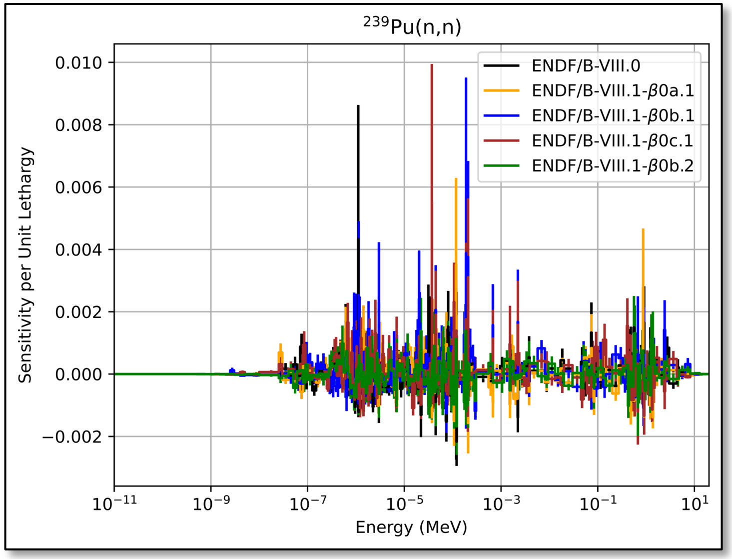
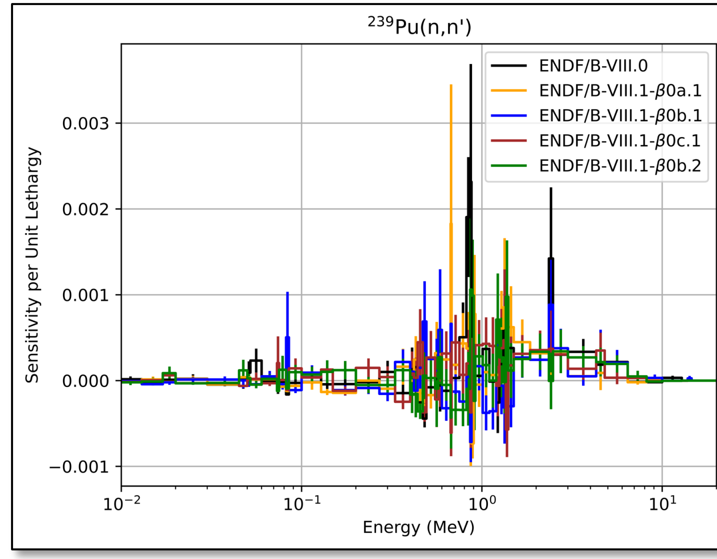
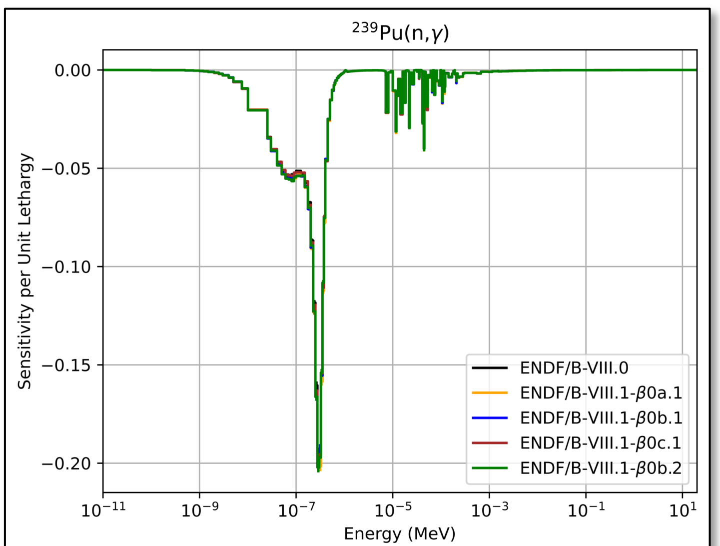
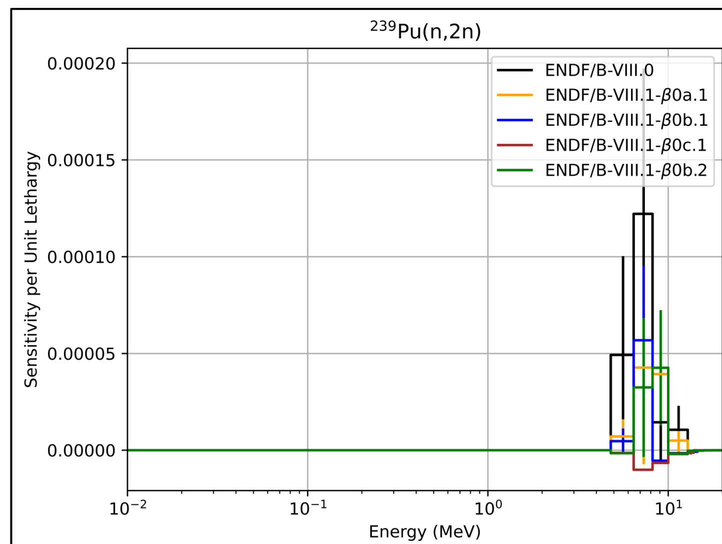
Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides, PU-SOL-THERM-034 Case 2 Benchmark ^{239}Pu Sensitivity









Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides, Jezebel & Godiva Reaction Rate Ratios

	C/E				
Reaction Rate Ratio* Jezebel	ENDF/B-VIII.0	ENDF/B-VIII.1-β0a.1	ENDF/B-VIII.1-β0b.1	ENDF/B-VIII.1-β0c.1	ENDF/B-VIII.1-β0b.2
^{169}Tm(n,2n)/^{235}U(n,f)	1.18933	1.13941	1.12747	1.16556	**1.12708**
^{191}Ir(n,2n)/^{235}U(n,f)	1.14892	1.10078	1.08910	1.12578	**1.08870**
^{238}U(n,2n)/^{235}U(n,f)	1.24899	1.20824	**1.20027**	1.23182	1.20248
^{238}U(n,f)/^{235}U(n,f)	0.99979	0.98351	0.99330	**1.00007**	0.99440
^{239}Pu(n,f)/^{235}U(n,f)	0.99817	0.99513	0.99599	**0.99830**	0.99624
Reaction Rate Ratio Godiva					
^{239}Pu(n,f)/^{235}U(n,f)	1.01800	**1.01685**	1.01714	1.01702	1.01714

*Reaction rate ratio measured values taken from Reference 3

Results – ENDF/B-VIII.0 $S(\alpha, \beta)$, ENDF/B-VIII-β0 nuclides, Flattop-Pu & Flattop-25 Reaction Rate Ratios

	C/E				
Reaction Rate Ratio Flattop-Pu	ENDF/B-VIII.0	ENDF/B-VIII.1-β0a.1	ENDF/B-VIII.1-β0b.1	ENDF/B-VIII.1-β0c.1	ENDF/B-VIII.1-β0b.2
^{169}Tm(n,2n)/^{235}U(n,f)	1.25283	1.20937	1.21469	1.23000	**1.19918**
^{191}Ir(n,2n)/^{235}U(n,f)	1.06656	1.03015	1.03437	1.04733	**1.02093**
^{203}Tl(n,2n)/^{235}U(n,f)	1.28912	1.24569	1.24887	1.26543	**1.23412**
^{238}U(n,2n)/^{235}U(n,f)	1.20523	1.17612	1.17587	1.19383	**1.17270**
^{238}U(n,f)/^{235}U(n,f)	1.04771	**1.03017**	1.03914	1.04840	1.04086
^{239}Pu(n,f)/^{235}U(n,f)	0.97694	0.97403	0.97468	**0.97719**	0.97493
Reaction Rate Ratio Flattop-25					
^{239}Pu(n,f)/^{235}U(n,f)	**0.98522**	0.98396	0.98428	0.98416	0.98428

Results – ENDF/B-VIII.0 $S(\alpha,\beta)$, ENDF/B-VIII-β0 nuclides, Neutron Reactor Kinetics Parameters

		C/E				
Metric*	**Benchmark**	ENDF/B-VIII.0	ENDF/B-VIII.1-β0a.1	ENDF/B-VIII.1-β0b.1	ENDF/B-VIII.1-β0c.1	ENDF/B-VIII.1-β0b.2
Prompt Neutron Decay Constant α	Jezebel	1.01591	**0.99934**	1.00420	1.02411	1.01617
	Flattop-Pu	**1.00035**	0.98457	0.98773	1.00533	0.99579
	Godiva	1.04467	**1.03323**	**1.03323**	**1.03323**	**1.03323**
	Flattop-25	1.05728	**1.04678**	**1.04678**	**1.04678**	**1.04678**
Effective Delayed Neutron Fraction β_{eff}	Jezebel	0.94845	0.94845	0.94845	0.95361	**0.95876**
	Godiva	**0.98786**	0.97724	0.97724	0.97724	0.97724

*Measured neutron reactor kinetics parameter values taken from Reference 4 and Reference 5

Conclusions

- A lot of results to digest…

- Benchmarks that don't include plutonium aren't changing as much, or in the direction we expect them to
- Plutonium benchmark results show a lot of promise – each Pu-239 file has qualities that make it desirable according to specific validation calculations – it would be beneficial to use the results shown in this presentation to design collaborative pathways forward
- Additional validation results are required to examine smaller trends for more conclusive statements

Acknowledgments

The validation work shown in these slides would not have been possible without the support and mentorship from Denise Neudecker and Skip Kahler. Skip Kahler not only produced some of the results shown in this presentation, but also helped to verify results. I would also like to acknowledge the hard work Nathan Gibson put into processing the ENDF-formatted files into ACE-formatted files that were used for all validation results shown and Wim Haeck for double checking all the produced ACE-formatted files.

The work performed at Los Alamos National Laboratory for this presentation was carried out under the auspices of the NNSA of the United States Department of Energy under contract 89233218CNA000001.

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