Criticality Data Testing at LANL with ENDF/B-VIII.1β1 Data Files

A. C. (Skip) Kahler and N. A. Kleedtke

XCP-5, Materials and Physical Data

Presented at the April 2023 Mini CSEWG Meeting

LA-UR-23-24422

ENDF/B-VIII.1β1 Criticality Data Testing

- Legacy LANL and Modern Critical Assemblies
  - Godiva, Jezebel, Flattop-25, Flattop-Pu, Big10, Jemima, Jezebel-23, Flattop-23.
  - KRUSTY, TEX
- HMF7
  - Multi-case suite with Energy of Average Lethargy causing Fission (EALF) ranging from low eV to hundreds of keV.
- Legacy HST suite
  - k_{calc} C/E correlation with Above-thermal Leakage Fraction (ATLF).

ENDF/B-VIII.1β1 Criticality Data Testing

- ^{233}U intermediate and thermal system assembly k_{calc} C/E correlated against Above-Thermal Fission Fraction (ATFF).
- PST suite
  - k_{calc} C/E correlation with ATLF and EALF.
- LCT
  - 509 assembly suite
  - Various reflectors
- Other, non-hydrogenous, reflected systems.

ENDF/B-VIII.1β1 Criticality Data Testing

- ENDF/B-VIII.1β1 Neutron Cross Section Files released on March 1, 2023.
  - Processed with NJOY2016.68.
    - Issue discovered with ^{9}Be low energy capture interpolation codes … corrected file used for data testing.

- ENDF/B-VIII.1β1.1 Thermal Scattering Law Files released on April 18, 2023.
  - Not yet processed.

- Any TSL data appearing in the benchmark results that follow used LANL processed data from the ENDF/B-VIII.0 “SaB2” Library.

Legacy LANL Critical Assemblies

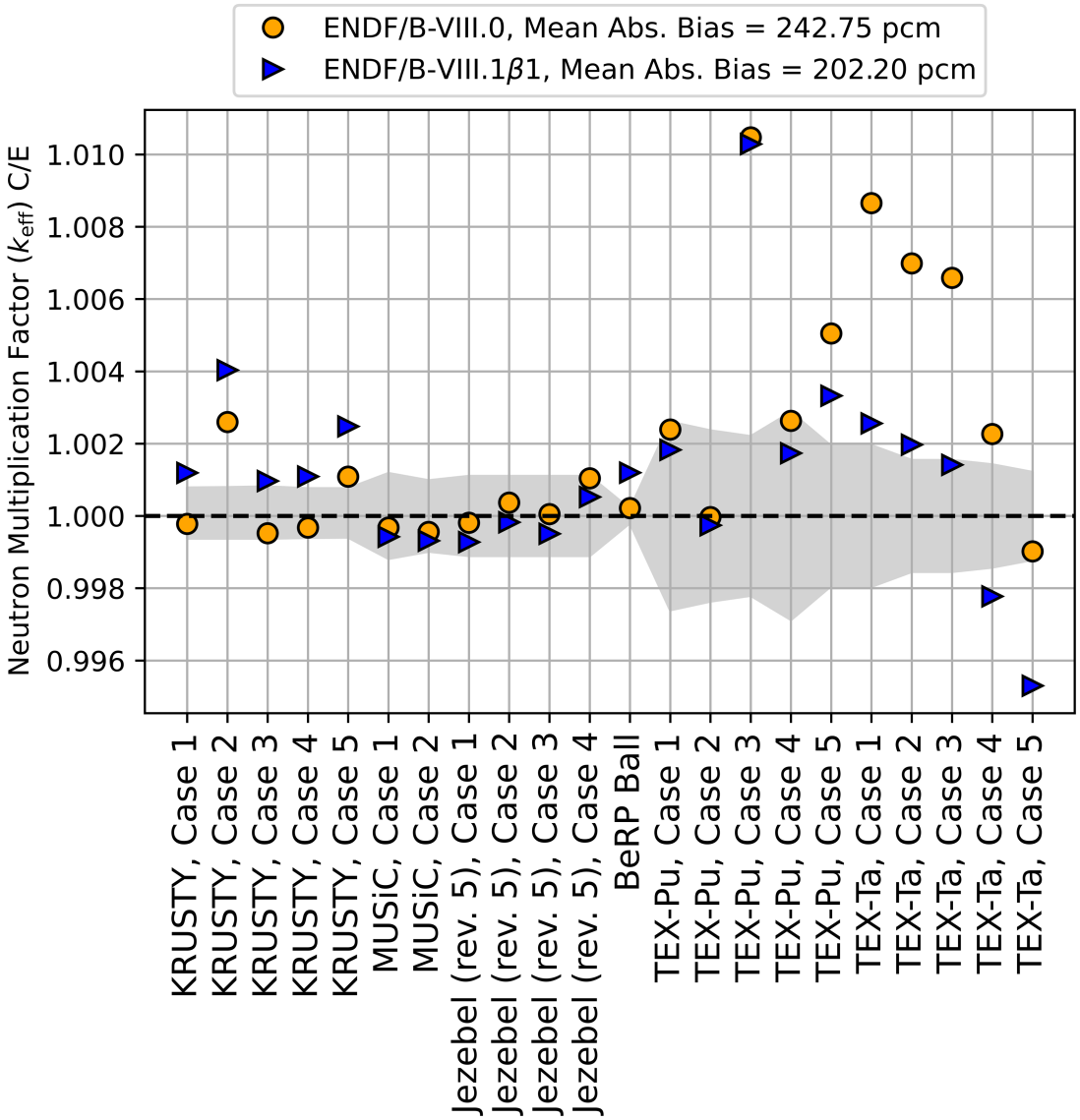
Fast, Bare (Godiva, Jezebel, Jezebel-23) remain as accurate, or better, than with ENDF/B-VIII.0 and earlier.

Flattops (-25, -Pu, -23) remain good.

Intermediate assemblies (Big-10, Jemima) are improved with the "pre-β2" ^{238}U candidate file.
- Big-10 ($k_{benchmark}$ = 1.0045) is as accurate as ever.
- Jemima has recovered from the small reactivity loss seen in e81β0 and e81β1 but remains less accurate than ENDF/B-VII.1

	NOTE: These are MCNP k_{calc} values, not C/E				
Benchmark	**E81β1 + pre- E81β2 ^{238}U**	E81β1	E81β02a	E80	E71
HMF1 (Godiva)	**0.99994(6)**	0.99991(4)	0.99993(4)	1.00007(4)	0.99977(6)
HMF28 (Flattop-25)	**1.00069(6)**	1.00054(4)	1.00061(4)	1.00080(4)	1.00270(6)
IMF1 (Jemima)	**0.99909(6)** **0.99932(6)** **0.99842(6)** **0.99961(6)**	0.99862(4) 0.99885(4) 0.99789(4) 0.99890(4)	0.99862(4) 0.99888(4) 0.99791(4) 0.99899(4)	0.99896(4) 0.99912(4) 0.99826(4) 0.99603(4)	1.00014(6) 1.00049(6) 1.00042(6) 1.00155(6)
IMF7 (Big-10)	**1.00451(5)**	1.00386(3)	1.00392(3)	1.00427(3)	1.00448(5)
PMF1 (rev5s)	**1.00001(6)**	1.00000(4)	1.00010(4)	1.00056(1)	---
PMF6 (Flattop-Pu)	**0.99971(7)**	0.99968(4)	0.99947(4)	0.99969(4)	1.00093(7)
UMF1	**1.00040(6)**	1.00038(4)	1.00008(4)	1.00045(4)	0.99986(6)
UMF6 (Flattop-23)	**1.00004(7)**	0.99990(4)	0.99935(4)	0.99999(4)	0.99887(7)

“Modern” Benchmark Suite Results

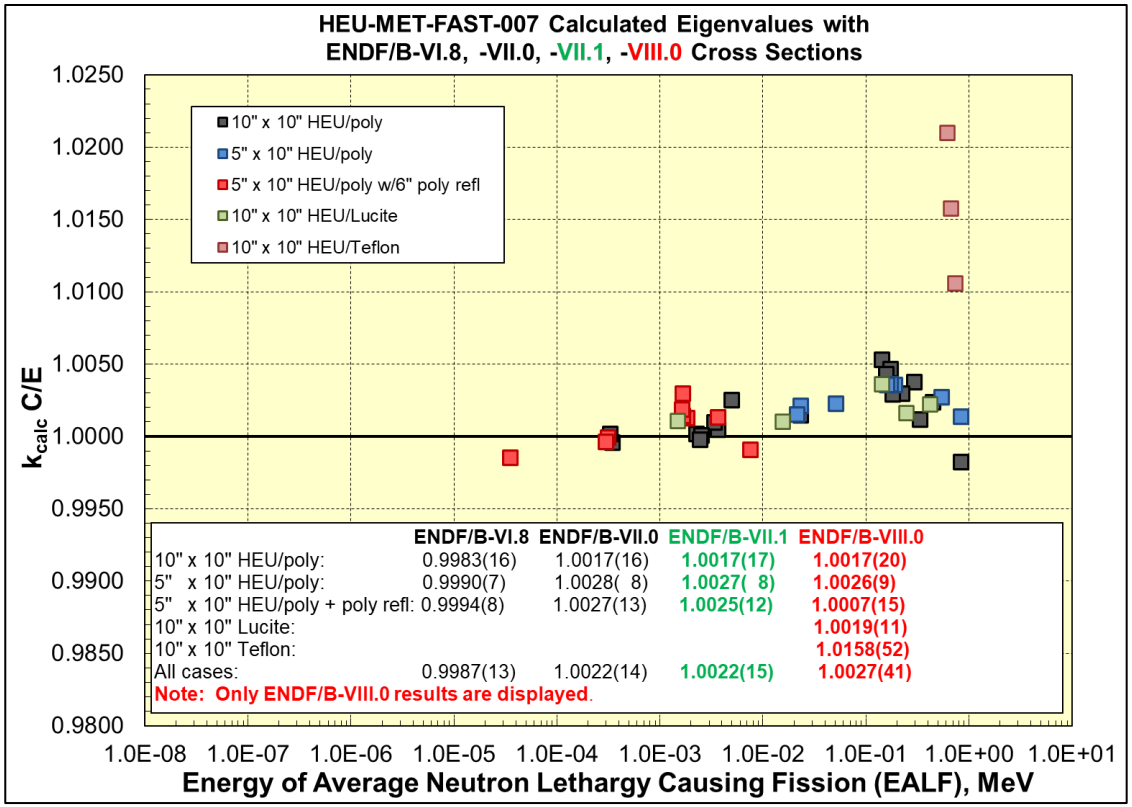


HMF7 vs EALF

Polyethylene and plexiglas reflected k_{calc} C/E results are mostly high with up to a several hundred pcm bias, plus exhibit a small trend (decreasing k_{calc} C/E with decreasing EALF).

- True for e70 and later.
- Similar shape with e68, but lower k_{calc} C/E.

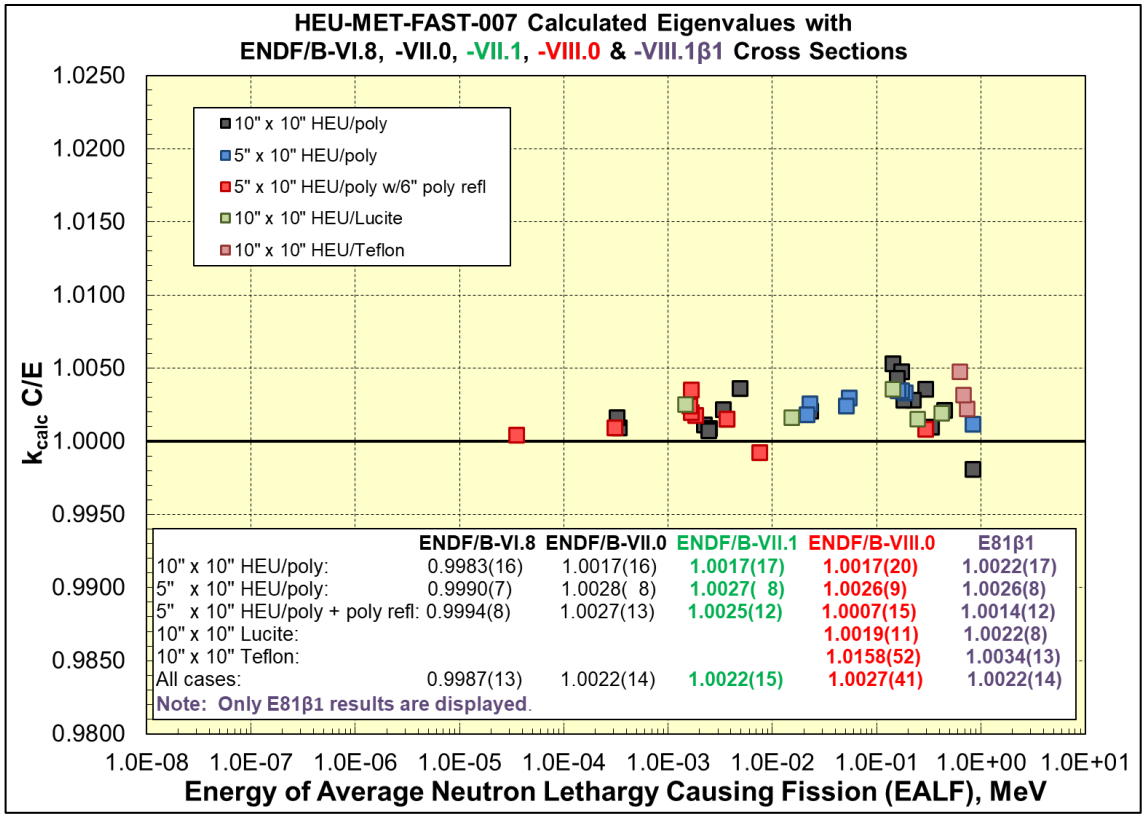
Teflon (^{19}F) reflected results are clearly deficient.



HMF7 vs EALF

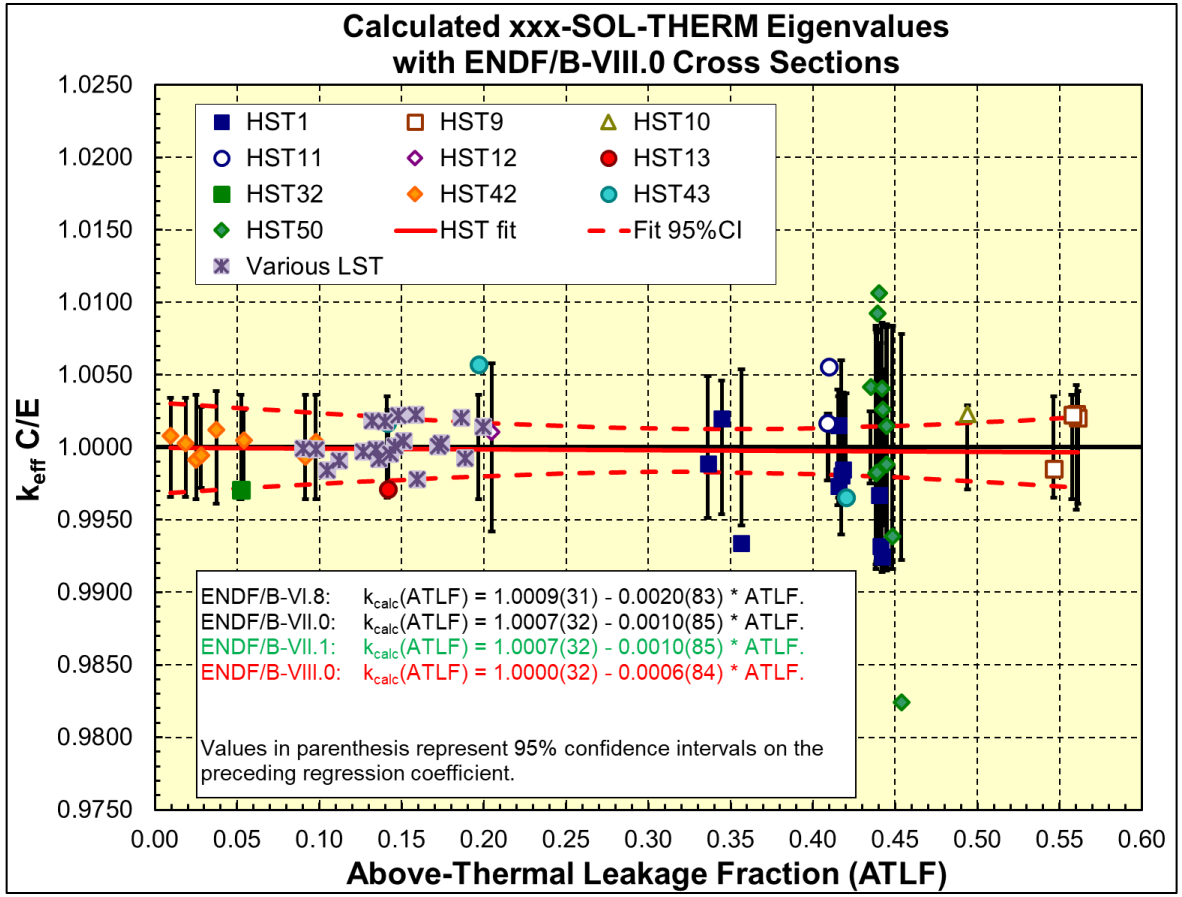
Polyethylene and plexiglas reflected k_{calc} C/E values are little changed from ENDF/B-VIII.0.

Teflon (^{19}F) reflected results are now consistent with polyethylene and lucite assemblies.



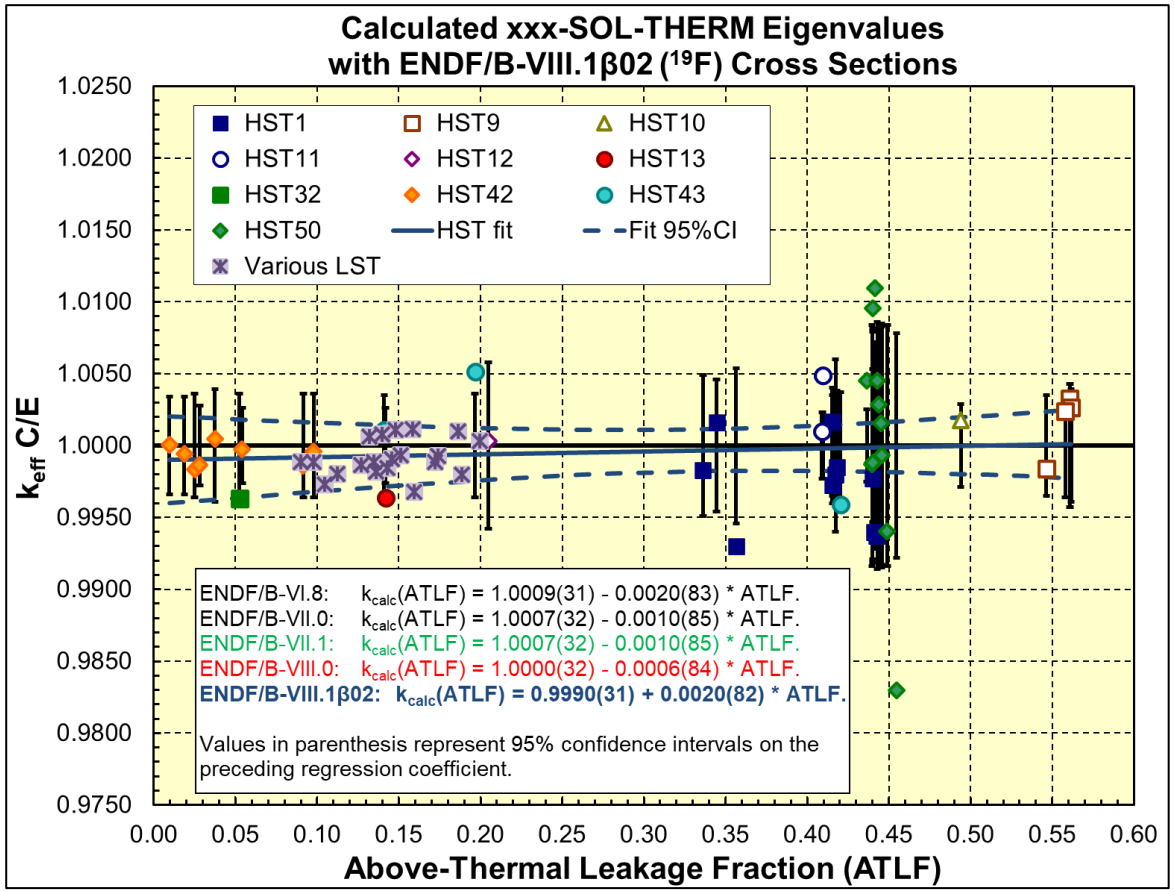
HST vs ATLF – ENDF/B-VIII.0

Starting point … unity intercept and zero slope, now seen for several generations of ENDF/B.



HST vs ATLF – ENDF/B-VIII.1β02

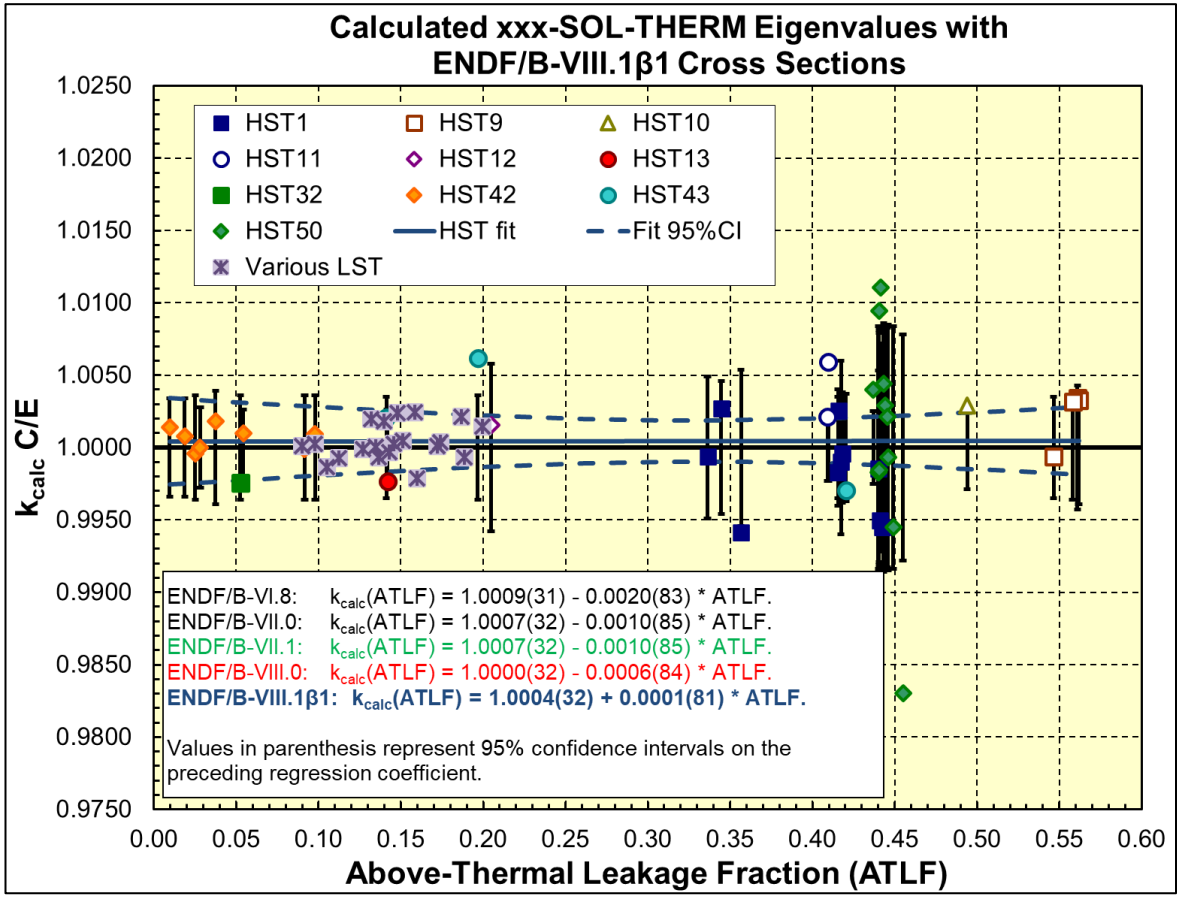
Unity intercept and zero slope, seen for several generations of ENDF/B, are retained … but change in intercept and slope parameters was larger than expected.



HST vs ATLF - ENDF/B-VIII.1β1

Unity intercept and zero slope, seen for several generations of ENDF/B, are retained.

Modest concern with e81β0 results has been eliminated.

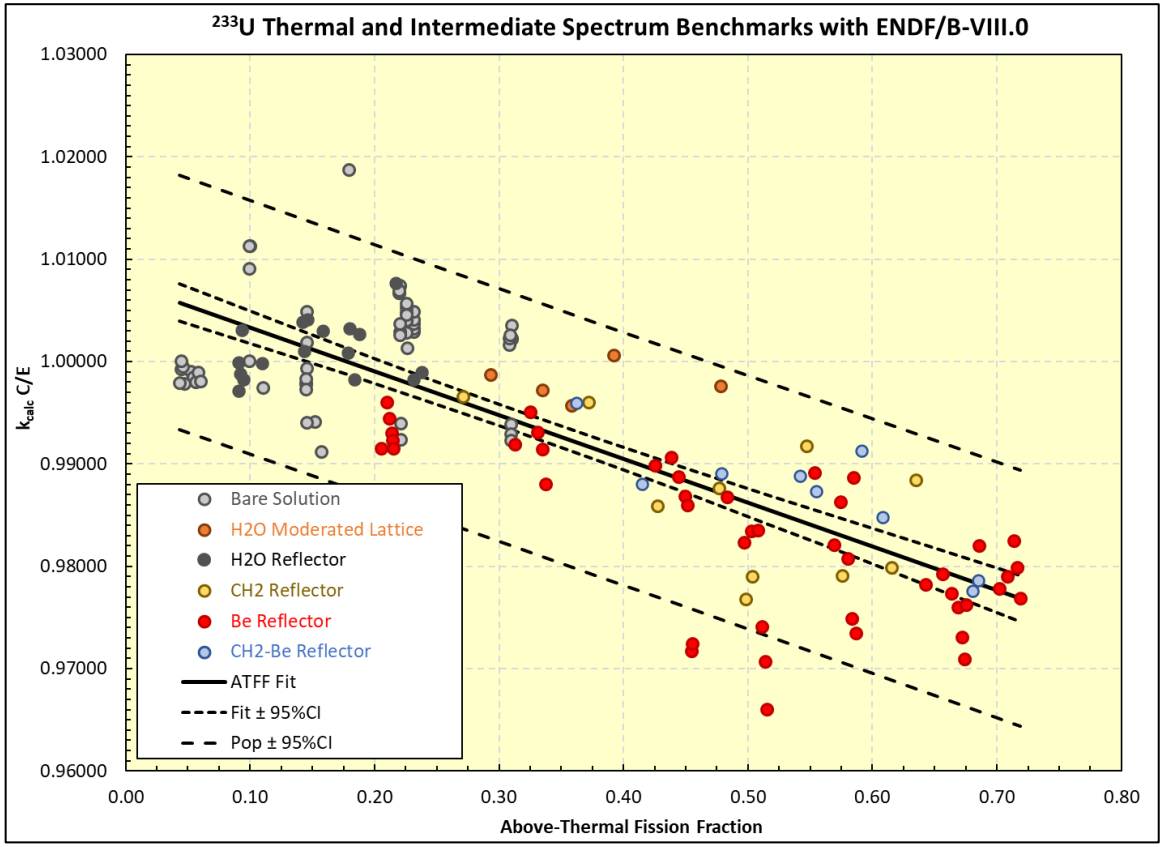


^{233}U – ENDF/B-VIII.0

Significant negative trend in k_{calc} C/E versus Above Thermal Fission Fraction (ATFF).

Lattice assemblies, from Naval Reactors LWBR Program, are calculated accurately … a successful demonstration reactor at Shippingport (1970s).

Minimal trend with bare and water reflected systems; severe drop-off with Polyethylene and Be reflected systems.



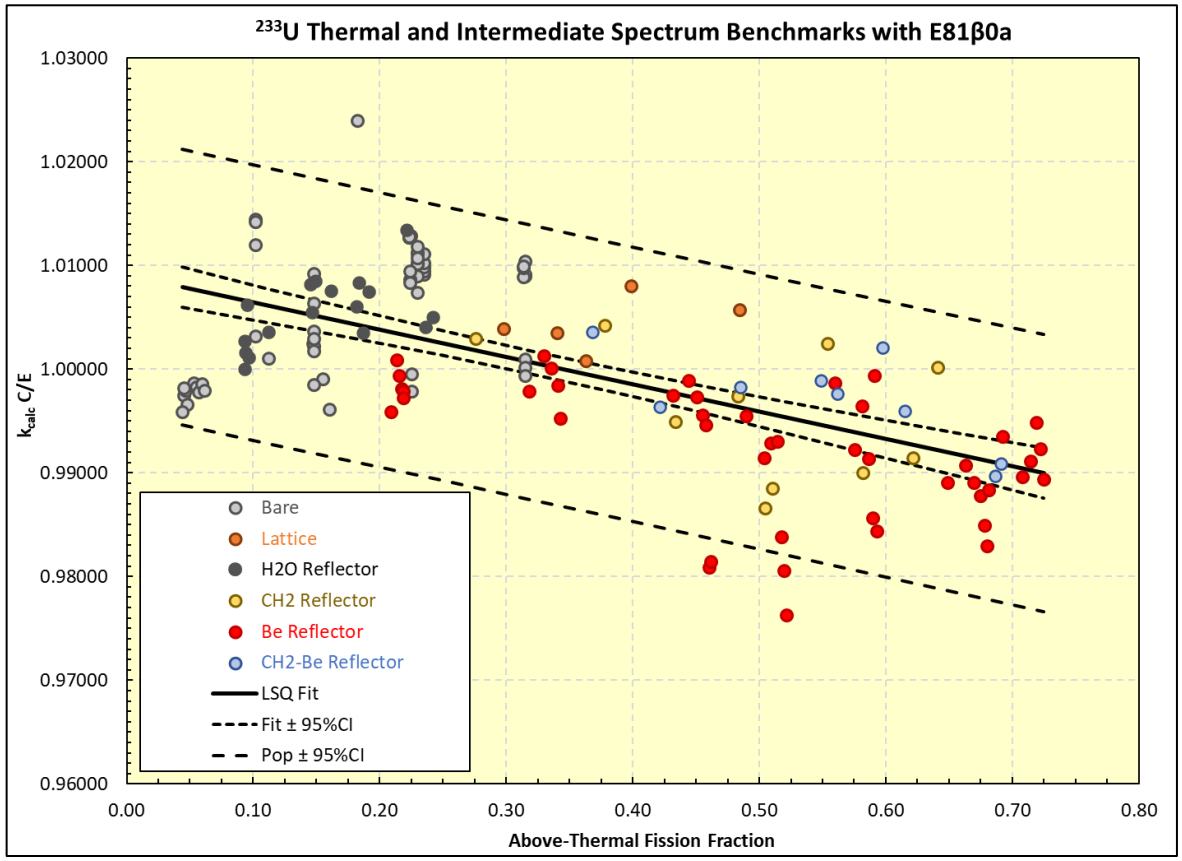
^{233}U – ENDF/B-VIII.1β0

INDEN (u233ornl_2b_nu6) ^{233}U evaluation.

Negative trend in k_{calc} C/E versus ATFF remains.

Lattice assemblies now biased high.

Positive trend for bare and water reflected systems masked by continuing negative trend at higher ATFF values for Polyethylene and Be reflected systems.

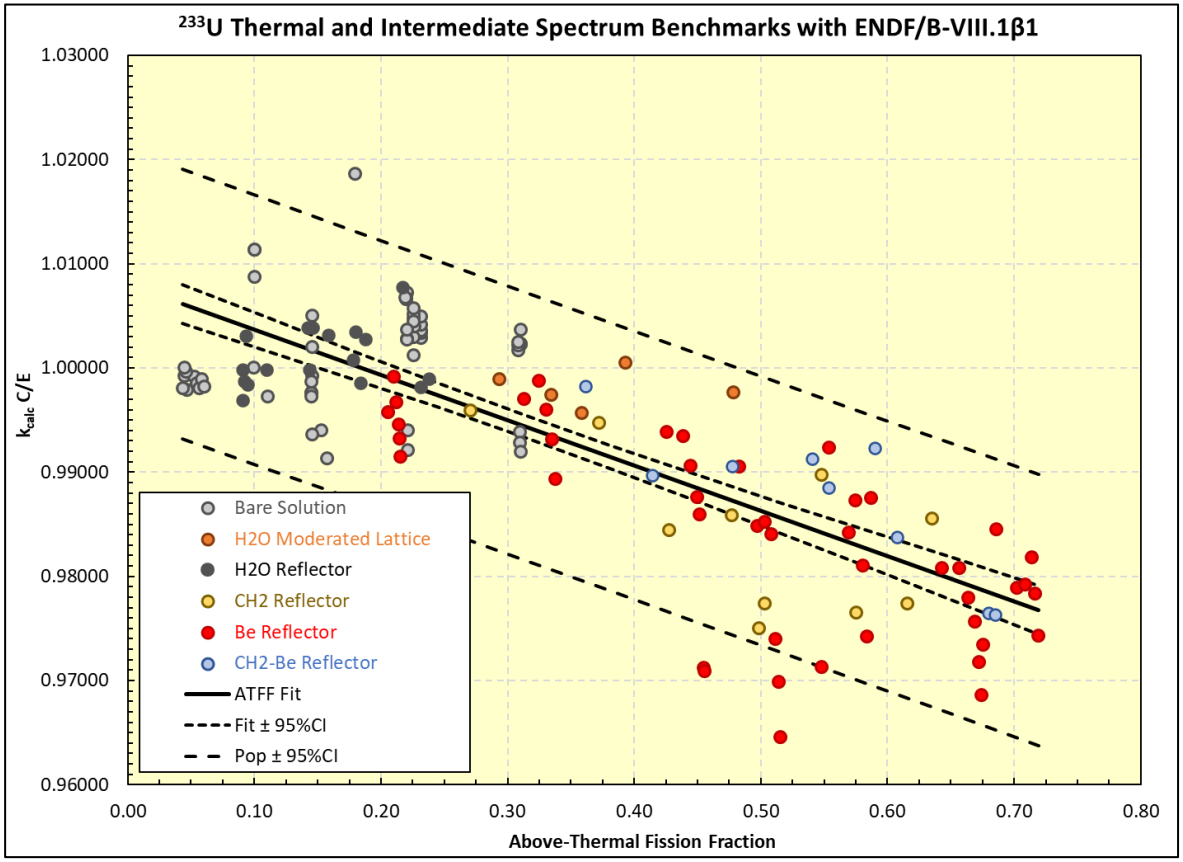


^{233}U – ENDF/B-VIII.1β1

Revert to ENDF/B-VIII.0 ^{233}U evaluation.

Changes to other nuclides have minimal impact on k_{calc} C/E.

Although ^{233}U is not a priority in the national scheme of things, there is clearly more work needed to more accurately characterize this nuclides nuclear data.

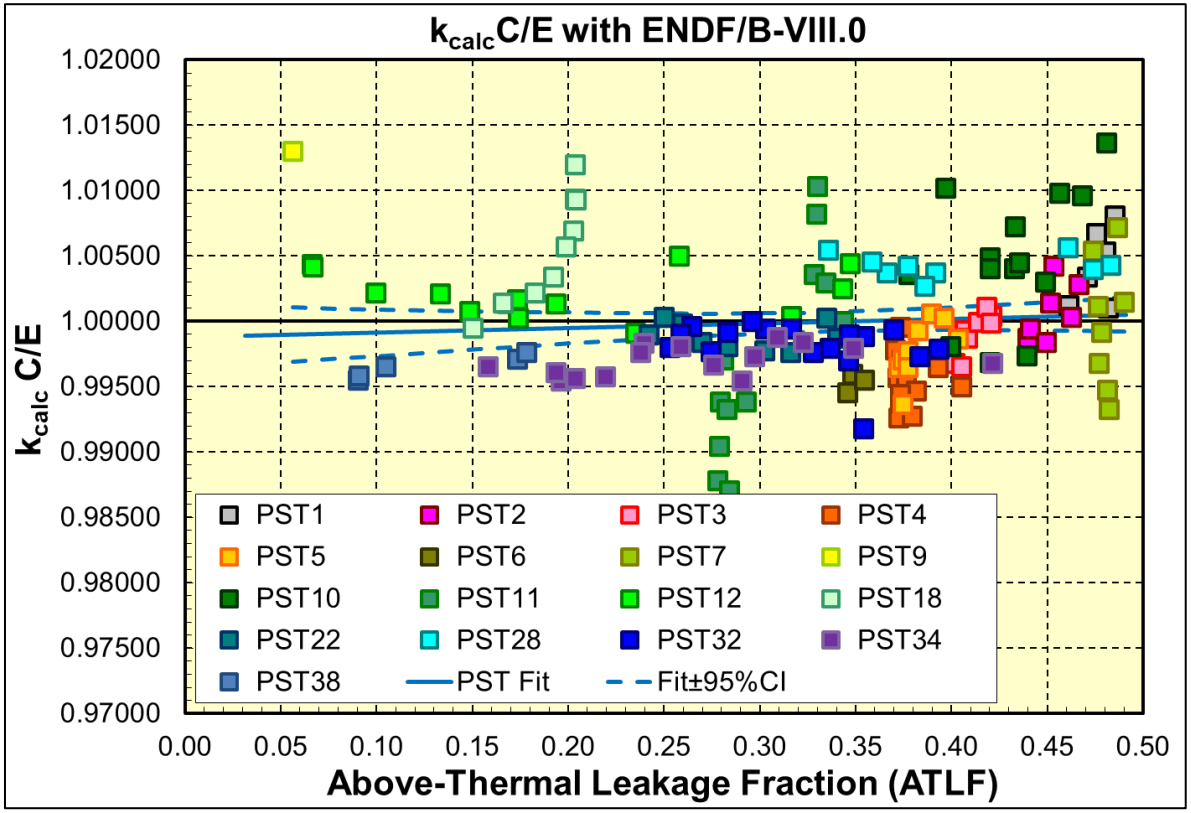


PST vs ATLF – ENDF/B-VIII.0

158 PST Assemblies

Possible trend with ATLF, but intercept and slope parameters are not statistically significant at the 95% confidence level.

Average k_{calc} C/E = 0.99996, but large standard deviation (468 pcm).



PST vs ATLF – ENDF/B-VIII.1β1

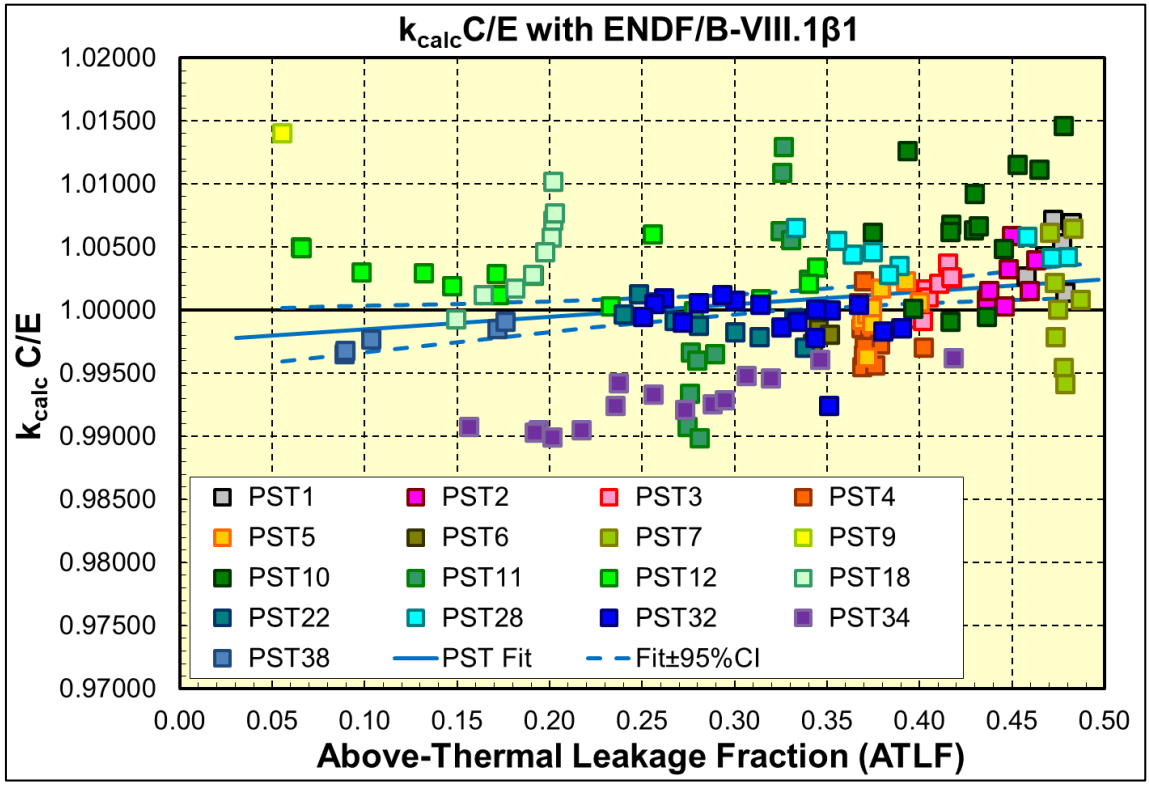
158 PST Assemblies

Average k_{calc} C/E = 1.00079, but large standard deviation (494 pcm).

Overall average has increased, but significant decrease in PST34 (Gd poisoned solution) results in a more prominent slope versus ATLF.

Seems like a Gd issue, but it's not seen in Gd poisoned LCT benchmarks.

The story continues …

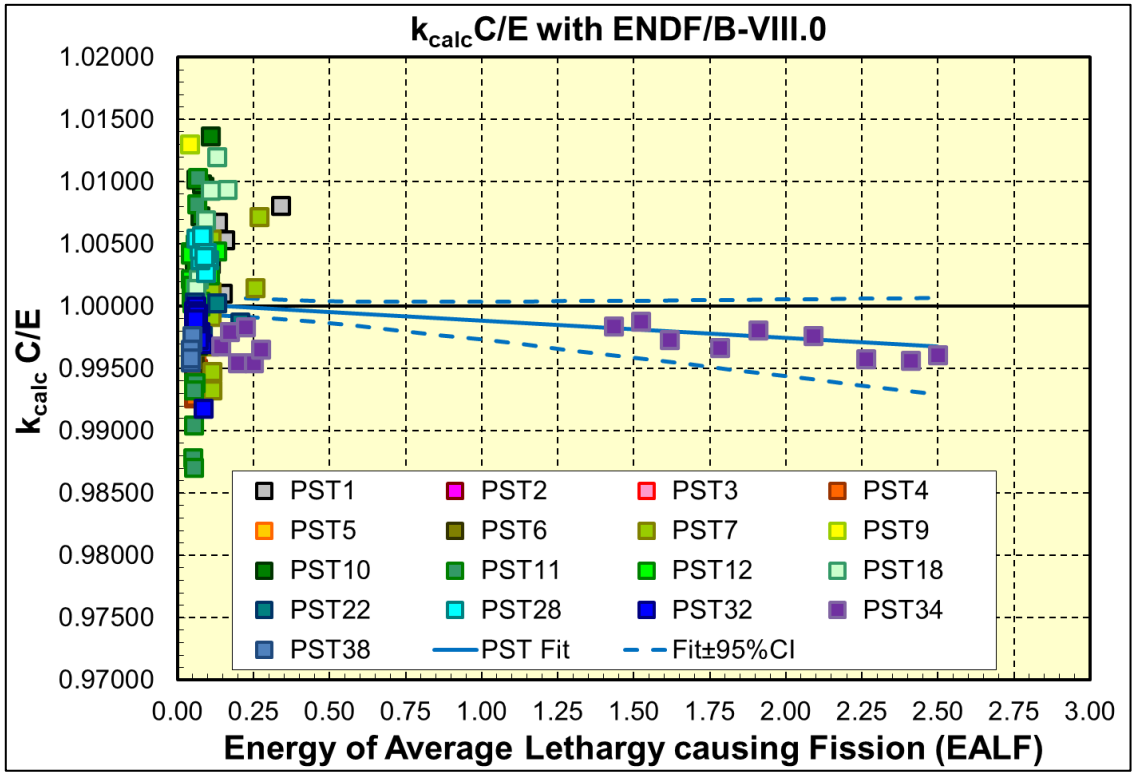


PST vs EALF – ENDF/B-VIII.0

In a recent conversation with Marco Pigni he asked if we'd looked at the PST calculations correlated against EALF (Energy of Average Lethargy causing Fission).
- the short answer was "not closely".

So here's what we see …

A cluster of points with EALF values below ~0.35 eV plus some PST34 configurations with much higher EALF values.
- As with ATLF the trend parameters are not statistically significant (95% CI).

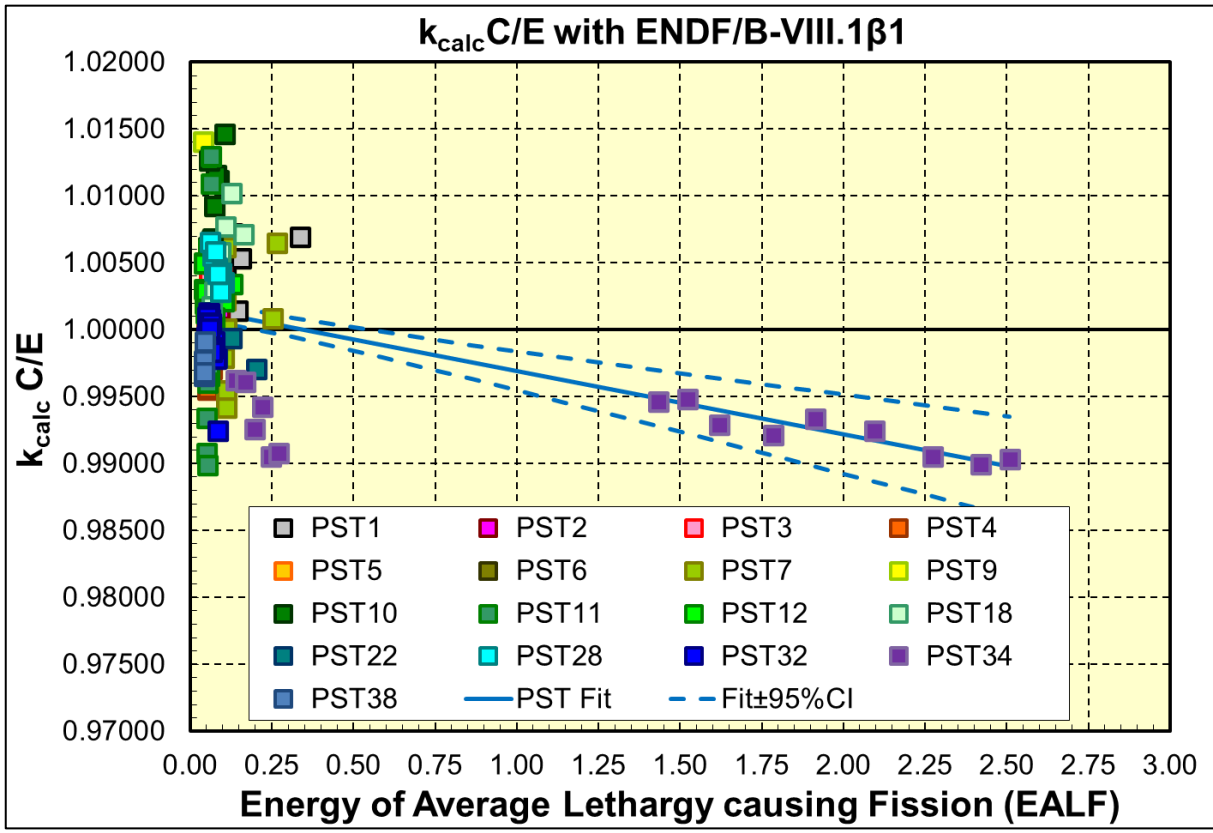


PST vs EALF – ENDF/B-VIII.1β1

Virtually all calculated eigenvalues have slightly increased (~100 pcm on average) except PST34 which exhibits an up to 500 pcm decrease.

But ^{239}Pu is a hybrid evaluation with components from multiple sources … INDEN/IAEA, LANL, LLNL, ORNL, … that previously existed in one or more of the e81β0a, e81β0b and e81β0c candidate files.

Looking back, e81β0a and e81β0b results are similar to what is seen here, but …

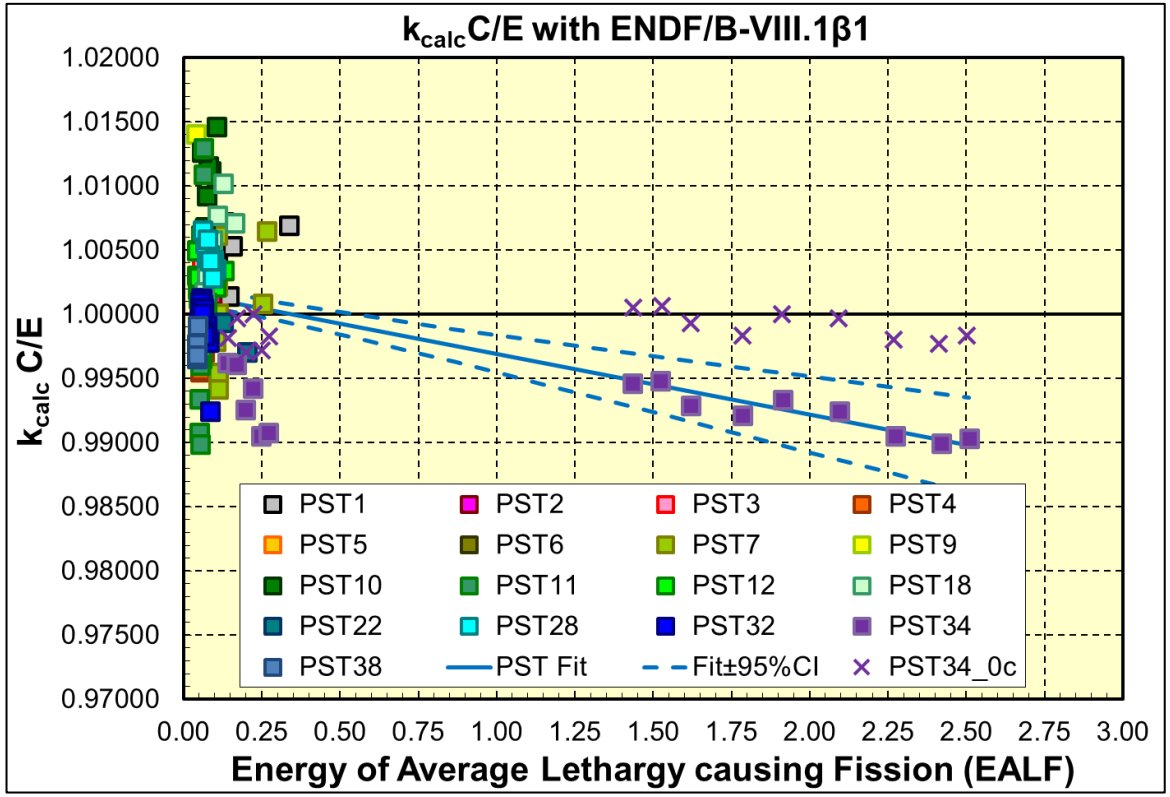


PST vs EALF – ENDF/B-VIII.1β1

Have superimposed PST34 results with e81β0c on the previous, e81β1, chart.

Only a few of the remaining PST assemblies have been calculated with e81β0c.
- Aside from PST34 the e81β0c results are about 100 pcm higher than obtained with E80.

Further review of the hybrid options in e81β1 ^{239}Pu seem warranted.

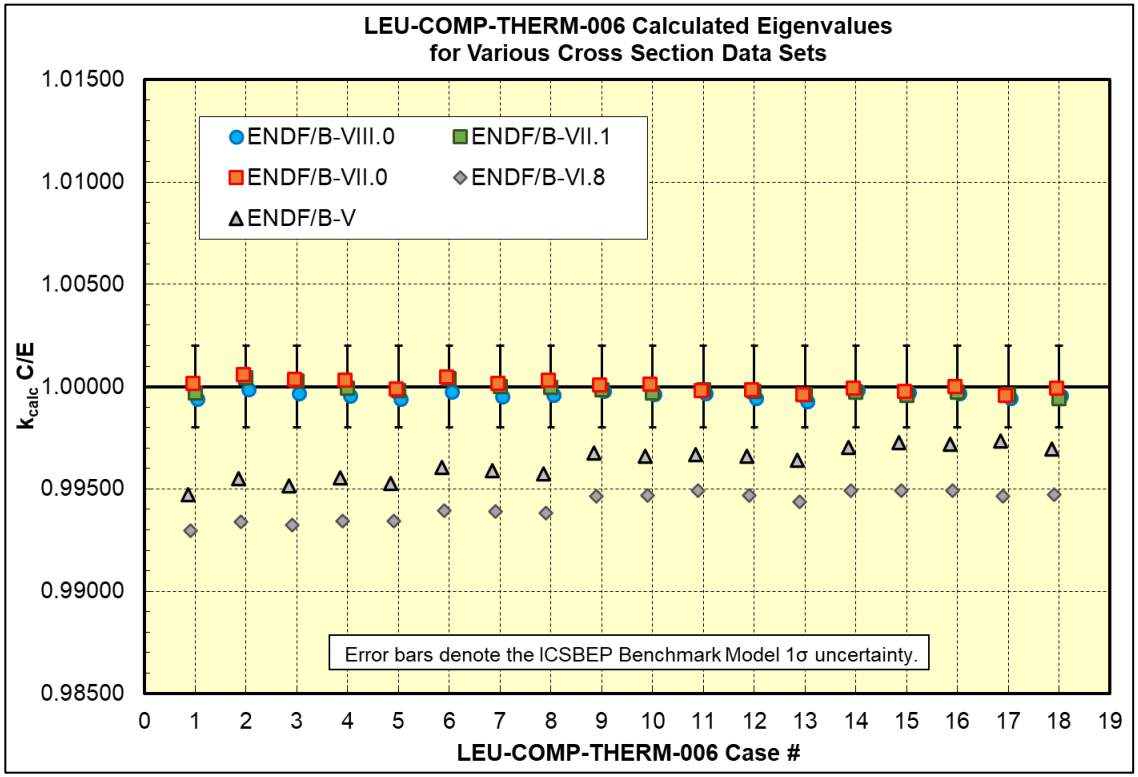


LCT – Various ENDF/B Generations

The LCT suite contains 509 assemblies.

The pattern shown by LCT6 is representative of the suite …

k_{calc} C/E (e5) = 0.99658 ± 0.00498
k_{calc} C/E (e68) = 0.99460 ± 0.00367
k_{calc} C/E (e70) = 0.99977 ± 0.00290
k_{calc} C/E (e71) = 0.99937 ± 0.00273
k_{calc} C/E (e80) = 0.99891 ± 0.00279



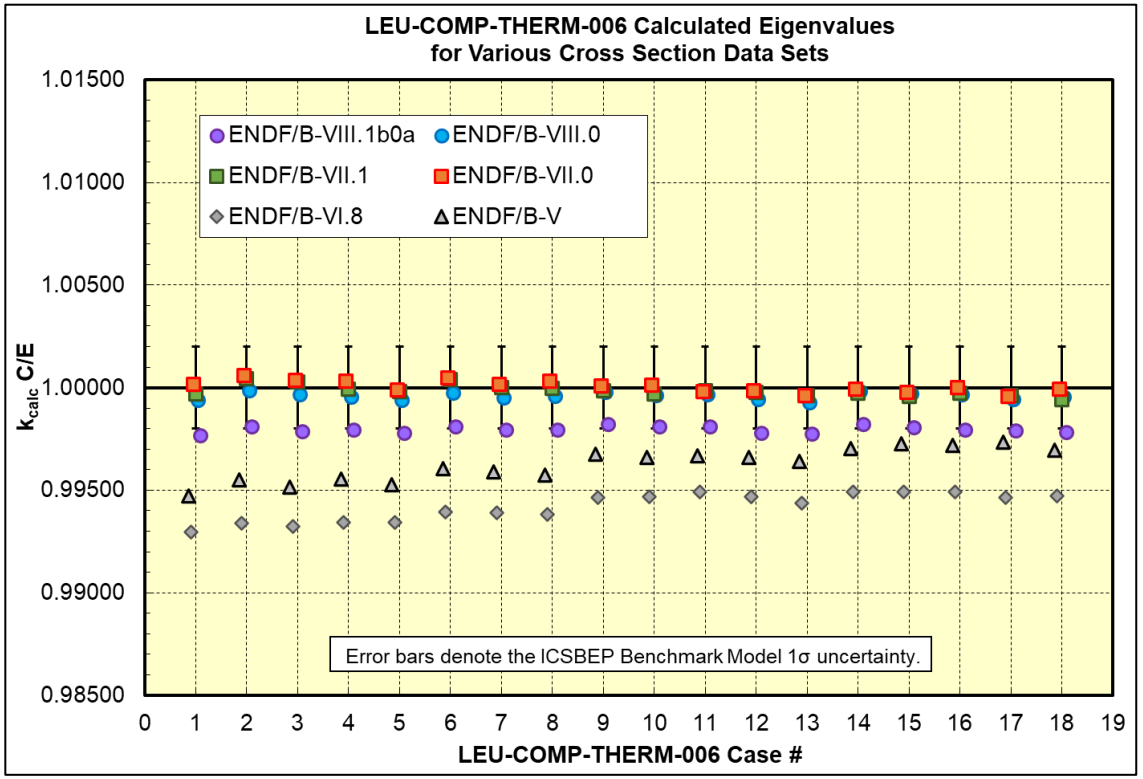
LCT – Various ENDF/B Generations

The LCT suite contains 509 assemblies.

The pattern shown by LCT6 is representative of the suite …

k_{calc} C/E (e5) = 0.99658 ± 0.00498
k_{calc} C/E (e68) = 0.99460 ± 0.00367
k_{calc} C/E (e70) = 0.99977 ± 0.00290
k_{calc} C/E (e71) = 0.99937 ± 0.00273
k_{calc} C/E (e80) = 0.99891 ± 0.00279
k_{calc} C/E (e81β0a) = 0.99770 ± 0.00275

- ~120 pcm reactivity loss from e80 (and over 200 pcm from e70) is concerning.

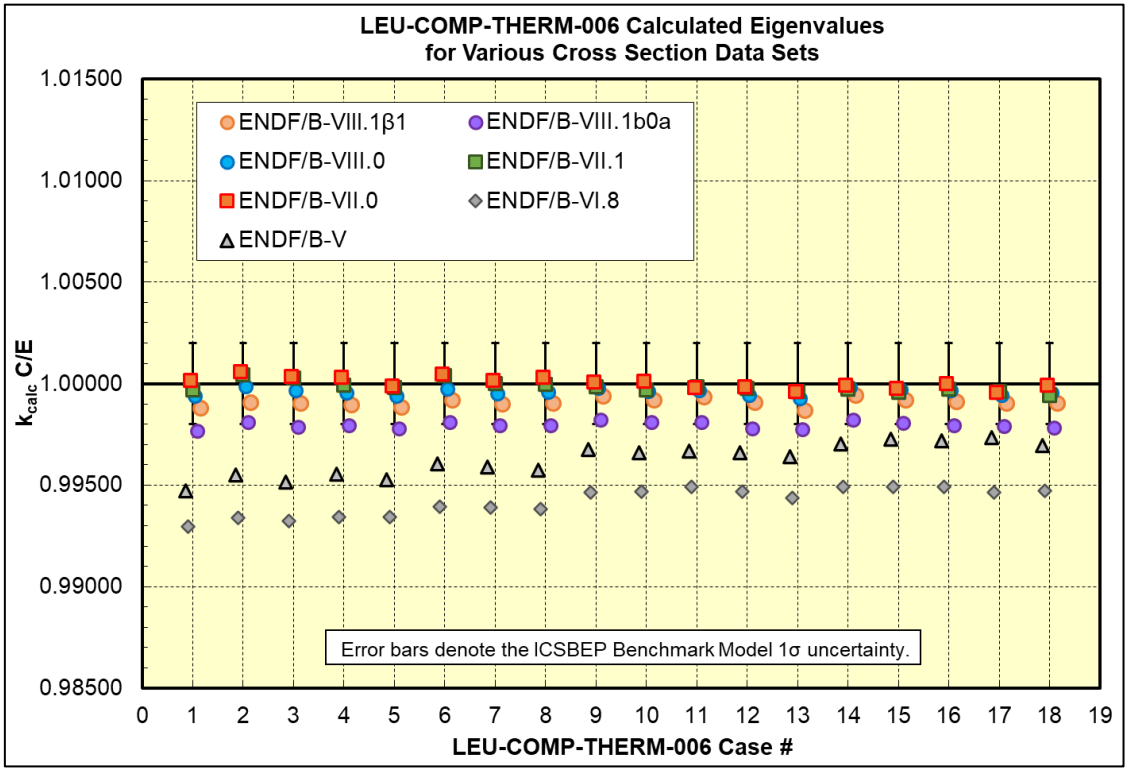


LCT – Various ENDF/B Generations

The LCT suite contains 509 assemblies.

The pattern shown by LCT6 is representative of the suite …

k_{calc} C/E (e5) = 0.99658 ± 0.00498
k_{calc} C/E (e68) = 0.99460 ± 0.00367
k_{calc} C/E (e70) = 0.99977 ± 0.00290
k_{calc} C/E (e71) = 0.99937 ± 0.00273
k_{calc} C/E (e80) = 0.99891 ± 0.00279
k_{calc} C/E (e81β0a) = 0.99770 ± 0.00275
k_{calc} C/E (e81β1) = 0.99871 ± 0.00275
- have recovered about half of the loss from e80.

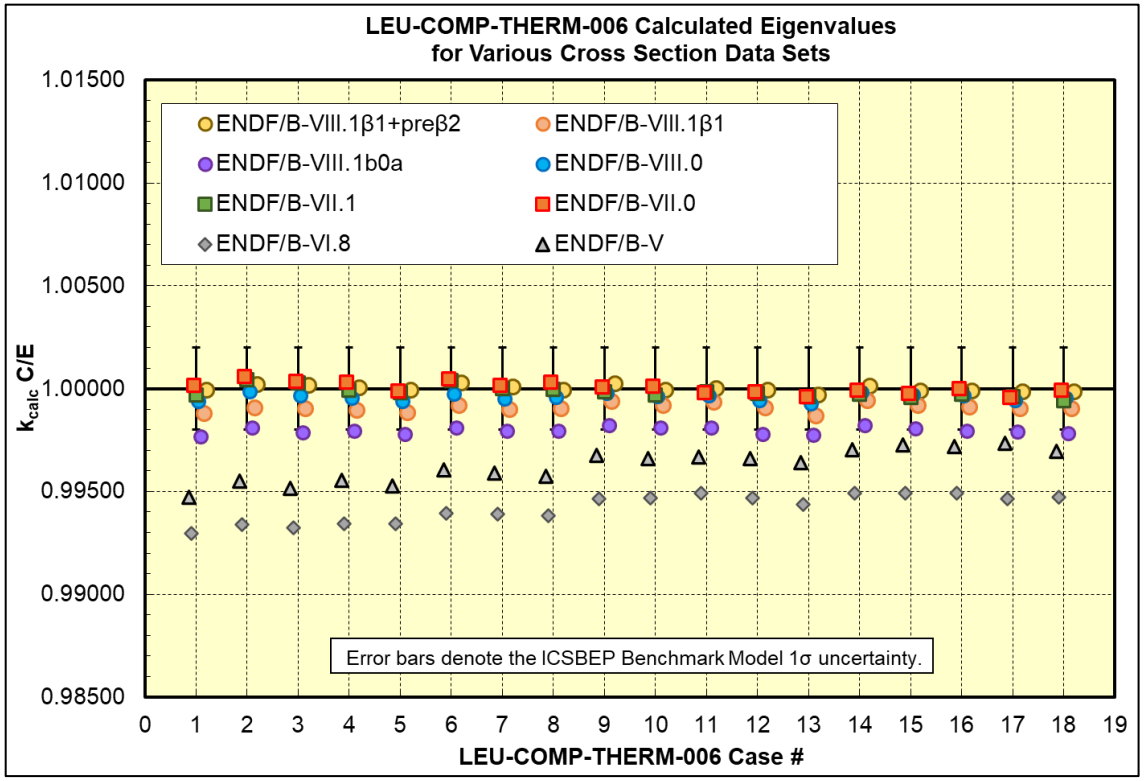


LCT – Various ENDF/B Generations

The LCT suite contains 509 assemblies.

The pattern shown by LCT6 is representative of the suite …

k_{calc} C/E (e5) = 0.99658 ± 0.00498
k_{calc} C/E (e68) = 0.99460 ± 0.00367
k_{calc} C/E (e70) = 0.99977 ± 0.00290
k_{calc} C/E (e71) = 0.99937 ± 0.00273
k_{calc} C/E (e80) = 0.99891 ± 0.00279
k_{calc} C/E (e81β0a) = 0.99770 ± 0.00275
k_{calc} C/E (e81β1) = 0.99871 ± 0.00275
k_{calc} C/E (e81preβ2) = 0.99953 ± 0.00274
- looking good, almost back to e70 level.



Be and Mix-Met-Fast-007

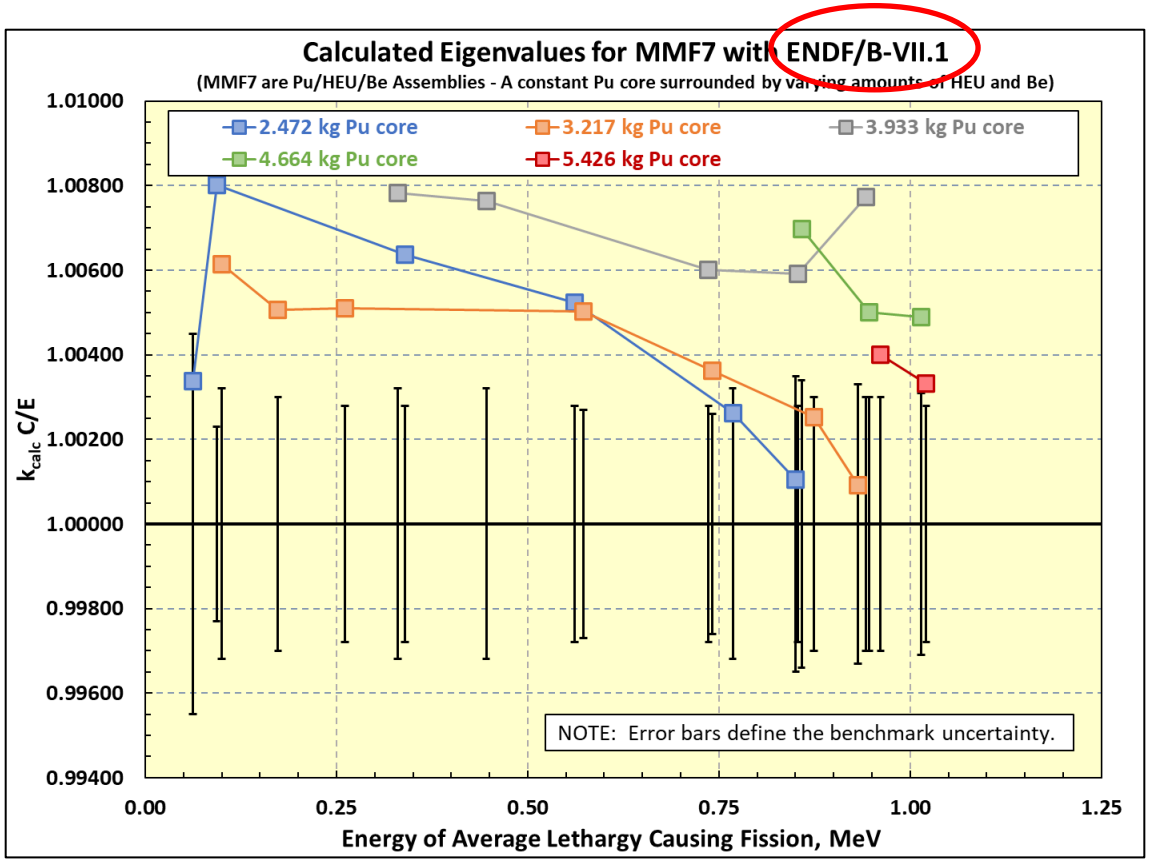
Fixed Pu core with HEU and Be reflectors

For a given Core start with a "small" HEU reflector then a "large" Be reflector

Each case, left-to-right, has a larger HEU component and a smaller Be component.

Leftmost data point for each core contains the most Be.

k_{calc} C/E is clearly biased high.



Be and Mix-Met-Fast-007

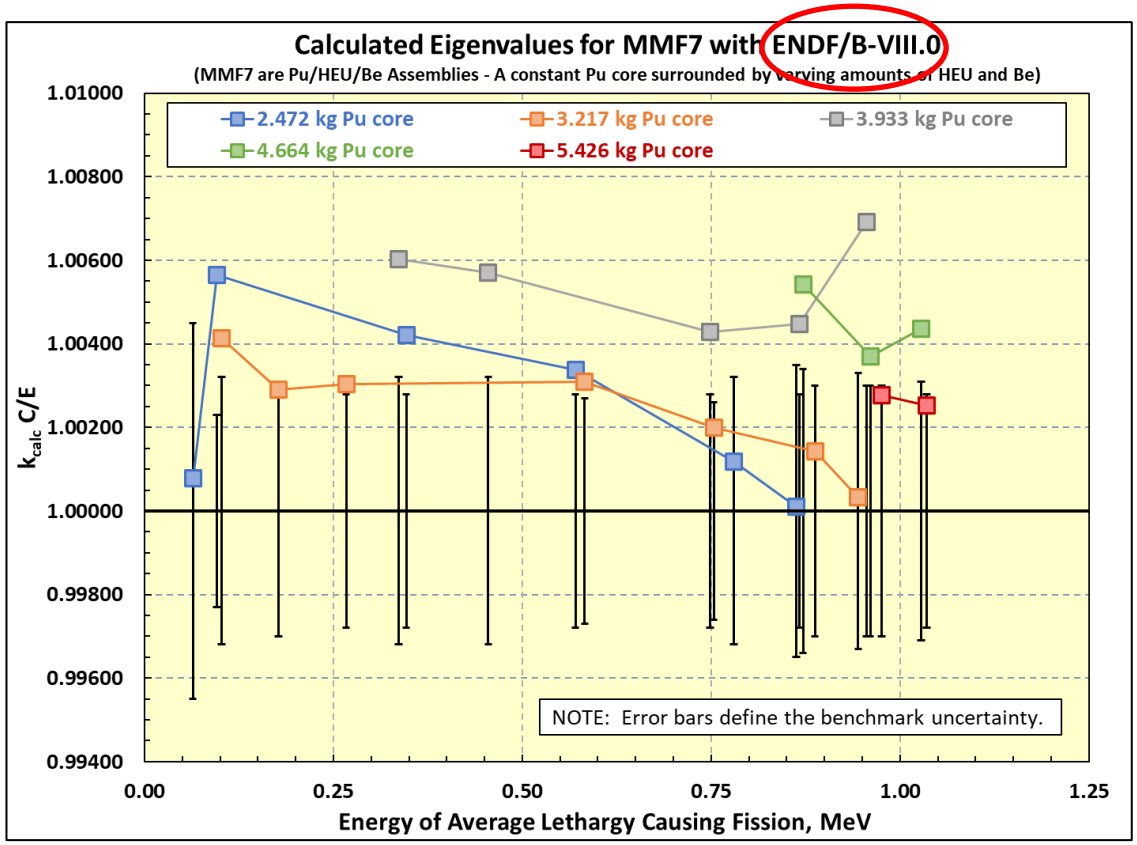
Fixed Pu core with HEU and Be reflectors

For a given Core start with a “small” HEU reflector then a “large” Be reflector

Each case, left-to-right, has a larger HEU component and a smaller Be component.

Leftmost data point for each core contains the most Be.

k_{calc} C/E is still biased high, but some improvement over ENDF/B-VII.1.



Be and Mix-Met-Fast-007

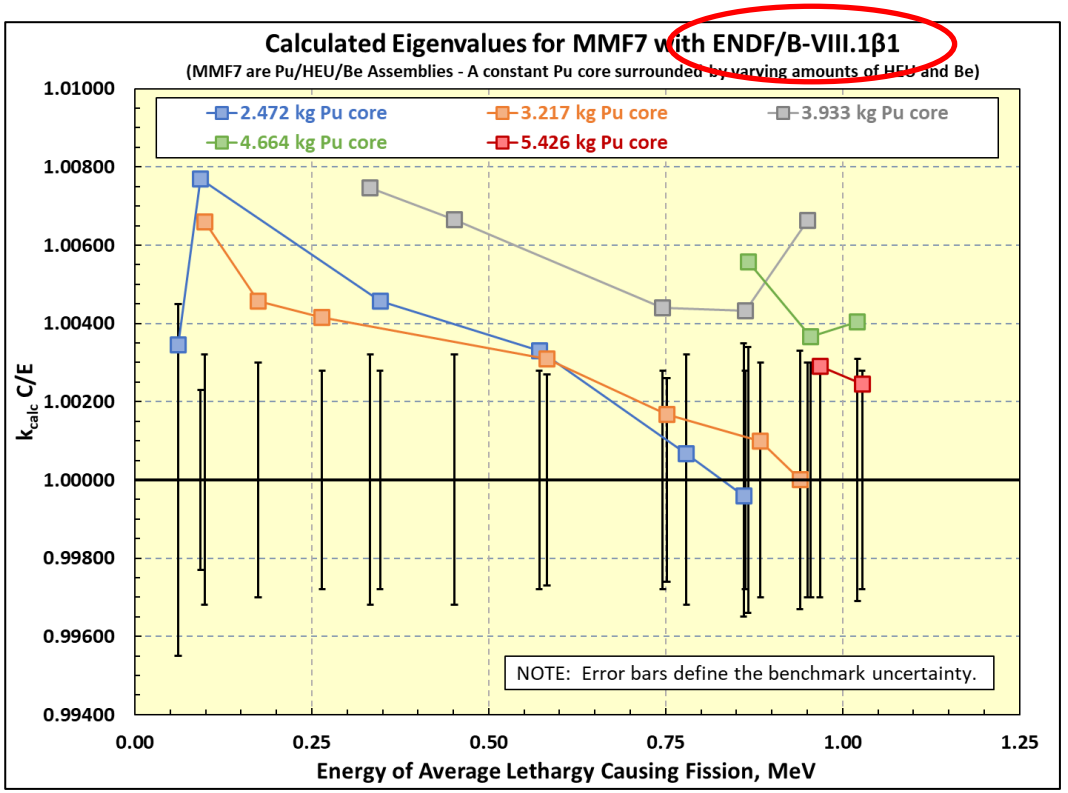
Fixed Pu core with HEU and Be reflectors

For a given Core start with a “small” HEU reflector then a “large” Be reflector

Each case, left-to-right, has a larger HEU component and a smaller Be component.

Leftmost data point for each core contains the most Be.

Seems like a step backwards as k_{calc} C/E remains biased high, but worse than ENDF/B-VIII.0 and closer to ENDF/B-VII.1 … but …



Be and Various HMFs

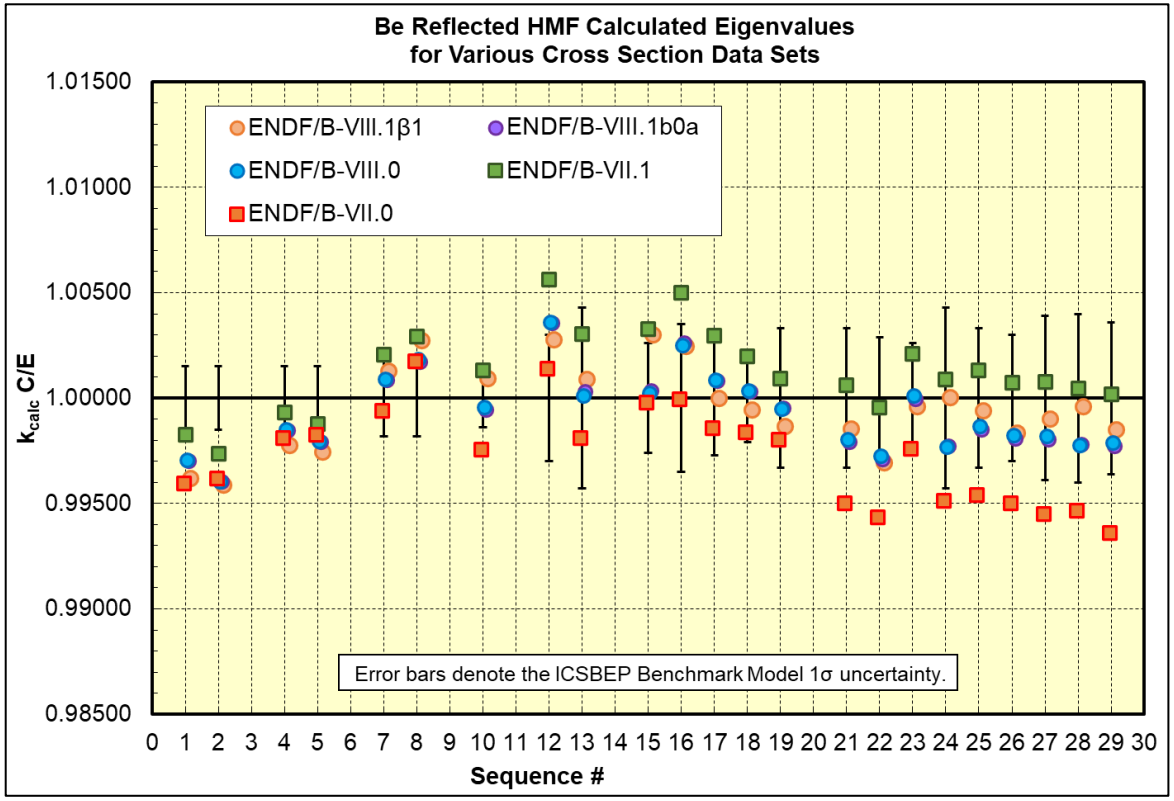
Results for ENDF/B-VII through today …

Benchmarks shown, from left-to-right include HMF9, HMF10, HMF16, HMF17, HMF41, HMF58 and HMF66.

E70 (reddish squares) is too cold …

E71 (green squares) is too hot …

E80 and E81 betas are in-between … no clear trend or reason to pick one over another.



Acknowledgments

Research reported in this publication was supported by the U.S. Department of Energy Advanced Simulation and Computing (ASC) program at Los Alamos National Laboratory. The authors would like to thank members of the LANL Nuclear Data Team for their help in processing and verifying ENDF/B-VIII.1β1 nuclear data files.