D. Rochman, M. Hursin and S.C. van der Marck

Adjustment of ^{239,240,241}Pu for the JEFF4T3 library

INDEN Meeting on Nuclear Data Evaluation of Fissile Actinides, IAEA, Vienna, 20-23 November 2023

Summary

- Method
- Adjustement
- Results
  - Updated cross sections / nubar
  - Verification
  - Validation (incl. crit-saf benchmarks, UO_2 and MOX reactivity)

Motivation and method

- Compared to JEFF-3.1.1, new libraries such as JEFF-3.3, JEFF-4T1, JEFF-4T2 have the following features
  - k_∞ reactivity loss and ^{239}Pu production loss
  - Mismatch with the standard thermal cross sections

- Goal: update Pu239, 240 and 241 to
  - Improve the reactivity curve and ^{239}Pu production with the VERA-1C Pincell model (56 + 55 points)
  - Be closer to the standards (4 points)
  - Check 18 PST criticality benchmark (18 points)
  - Check kritz benchmarks (2 points)
  - Check the alpha ratio (18 Points)
  - (in total, 153 points)

Motivation and method

- Method:
  - GLLS on group nubar for Pu239 with 14 energy groups from 0 to 16 eV: 14 parameters

0-0.01 eV	0.01-0.03	0.03-0.06	0.06-0.1	0.1-0.14
0.14-0.19	0.19-0.30	0.30-0.35	0.35-0.625	0.625-2.0
2.0-4.0	4.0-6.525	6.525-6.825	6.825-16.0	

  - GLLS on resonance parameters for the 3 isotopes
    - Pu239: Γ_n, Γ_γ, Γ_{f1} and Γ_{f2} for the 24 first resonances (-70 to 50 eV): 96 parameters
    - Pu240: Γ_n, Γ_γ, Γ_f for the 9 first resonances (-4071-6.66 eV): 27 parameters
    - Pu241: Γ_n, Γ_γ, Γ_{f1} and Γ_{f2} for the 47 first resonances (-59.5 to 48.1 eV): 188 parameters
  - In total: 14+96+27+188= 325 parameters

Validation

- Validation: Compare the prior (JEFF-4T2) and the updated Pu239, 240, 241 for systems not included in the GLLS adjustement
  - UO_2 and MOX pincells
  - Other criticality experiments
  - Duke PWR benchmark

Model for the pincell calculation (reactivity effect)

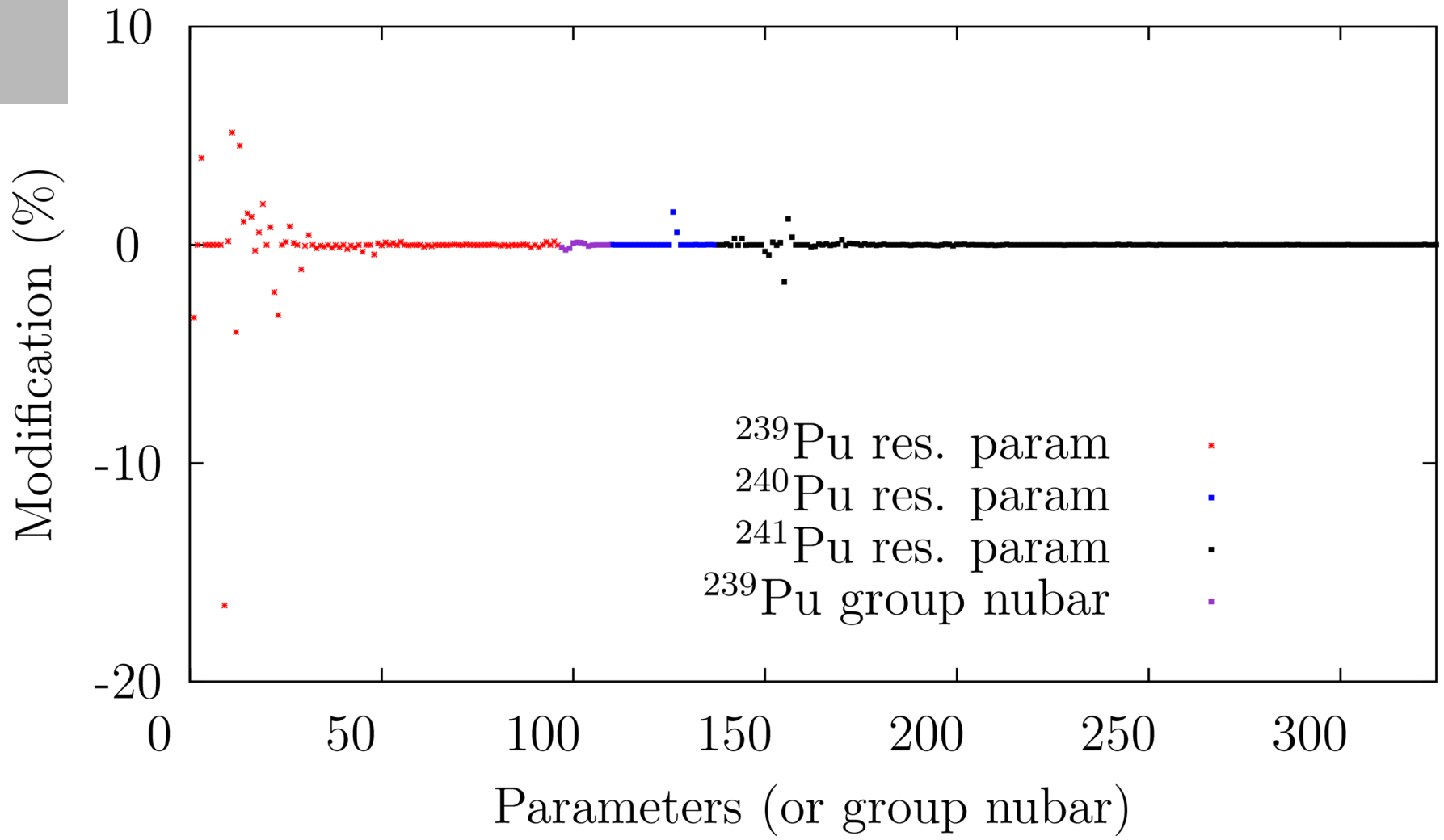
- VERA-1C Pincell model (3.1% enrichment / 1300 ppm / HFP conditions)
  - Watts Bar Nuclear 1 Cycle 1 maximum enrichment
  - Specs from the CASL-U-2012-0131-002 report

- Dragon Calculation options

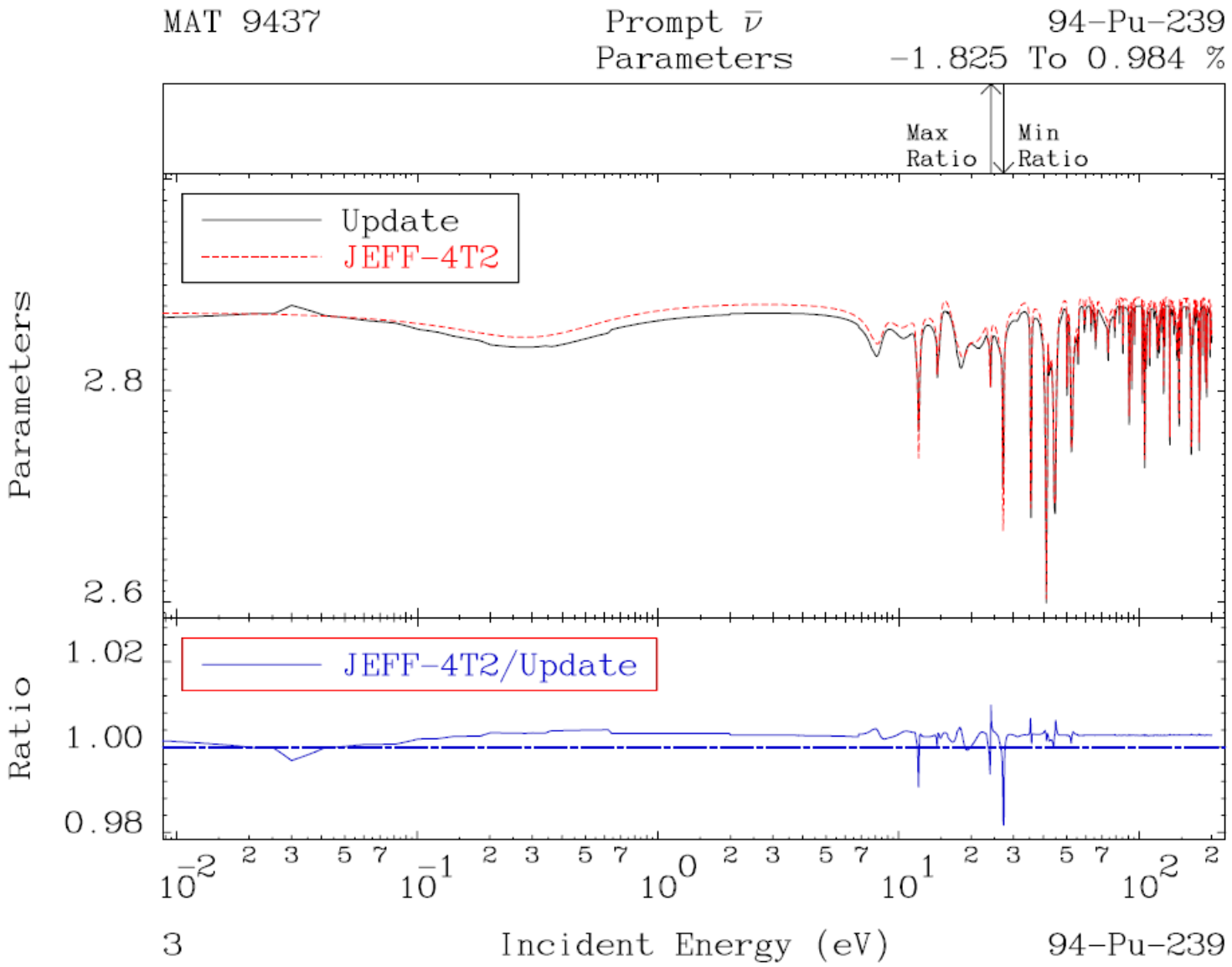
Library format	WIMSD-172
Resonance method	Subgroup
Self-shielding	Pin-averaged
Transport method	MOC

Impact on resonance parameters and nubar

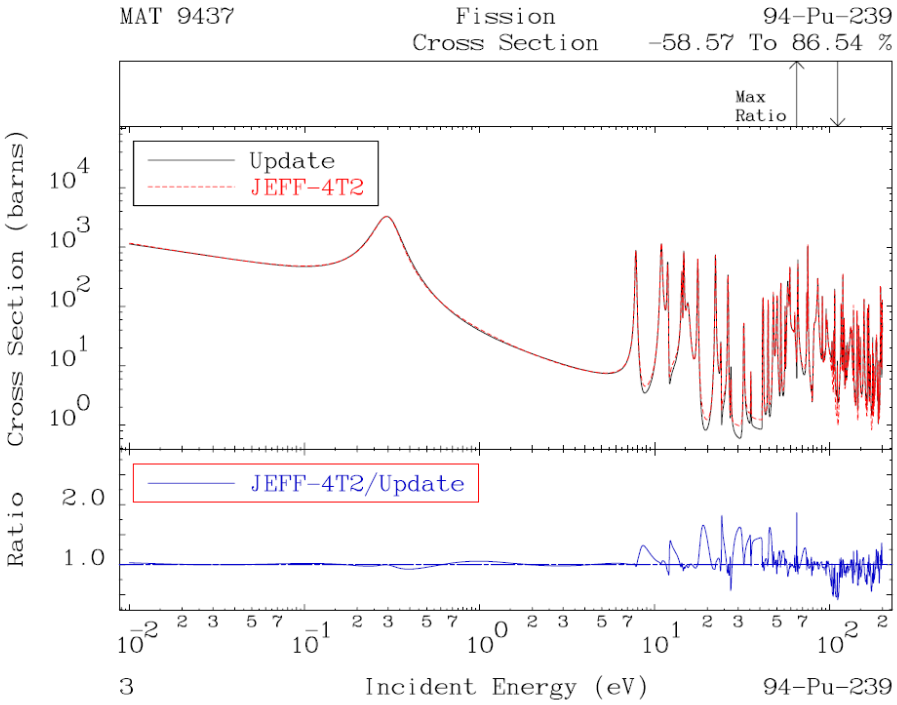
- After GLLS, parameters are modified:

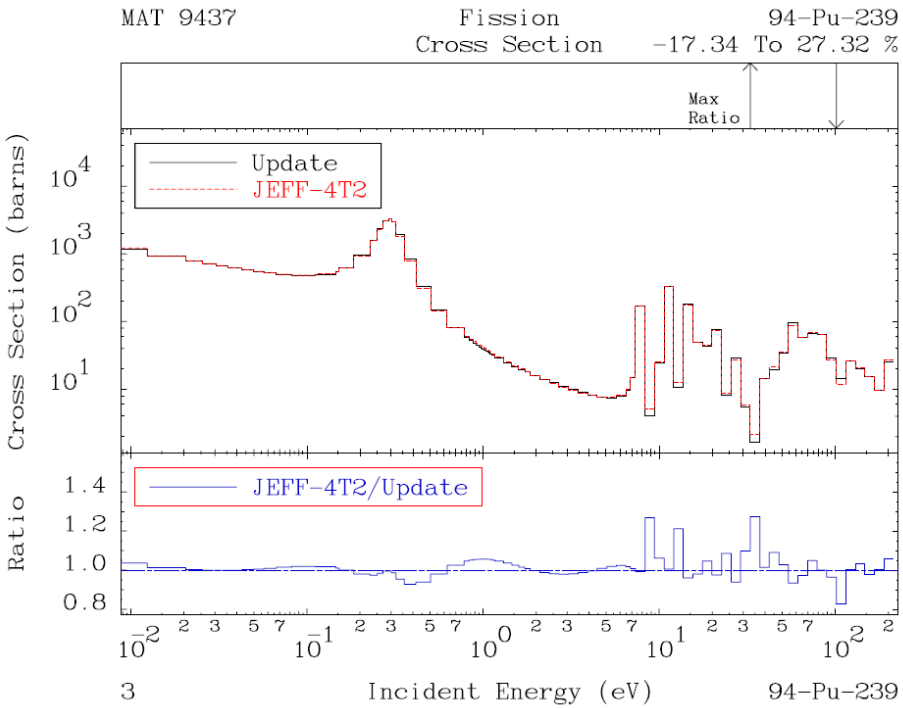


Impact of GLLS on ^{239}Pu nubar

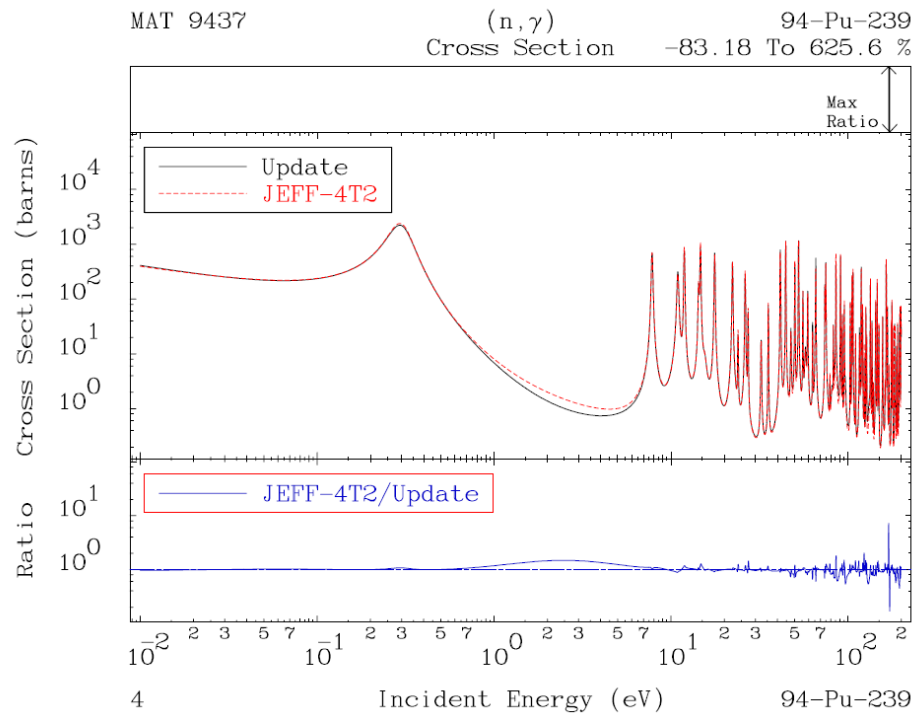


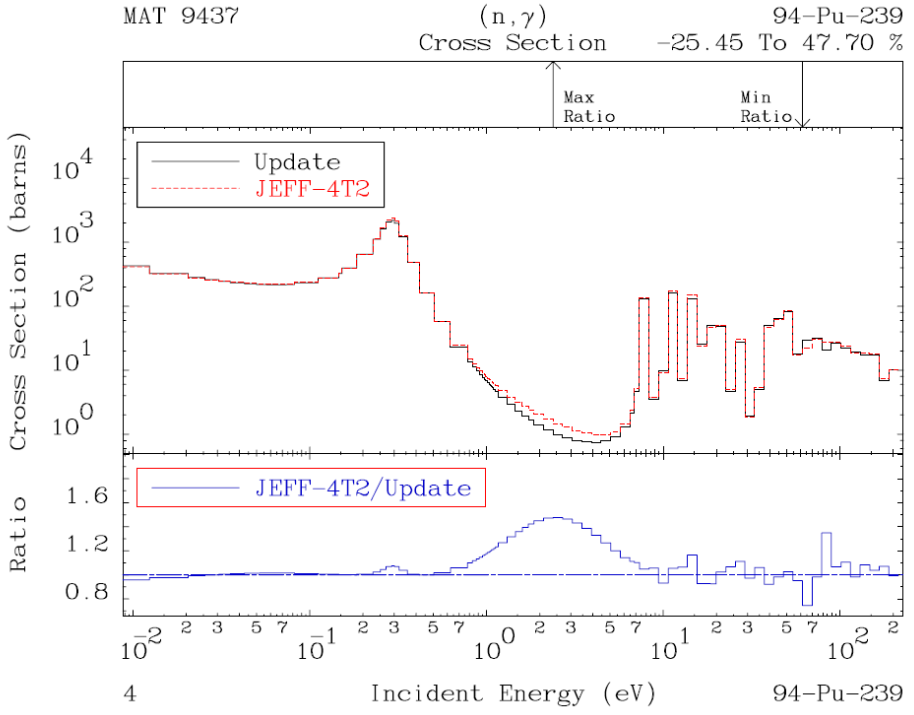
Impact of GLLS on ^{239}Pu(n,f) cross section



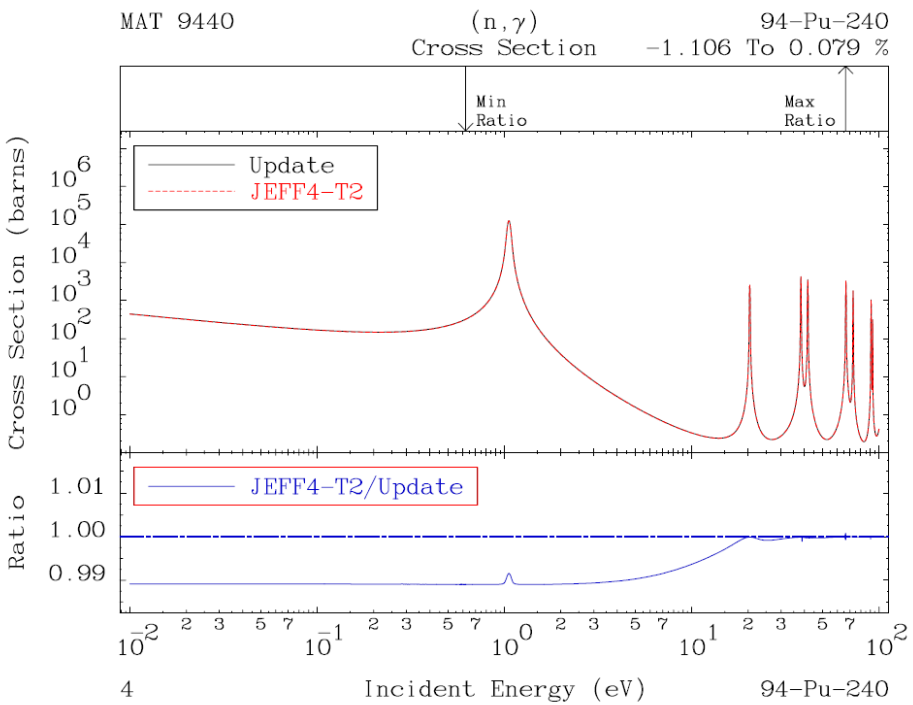


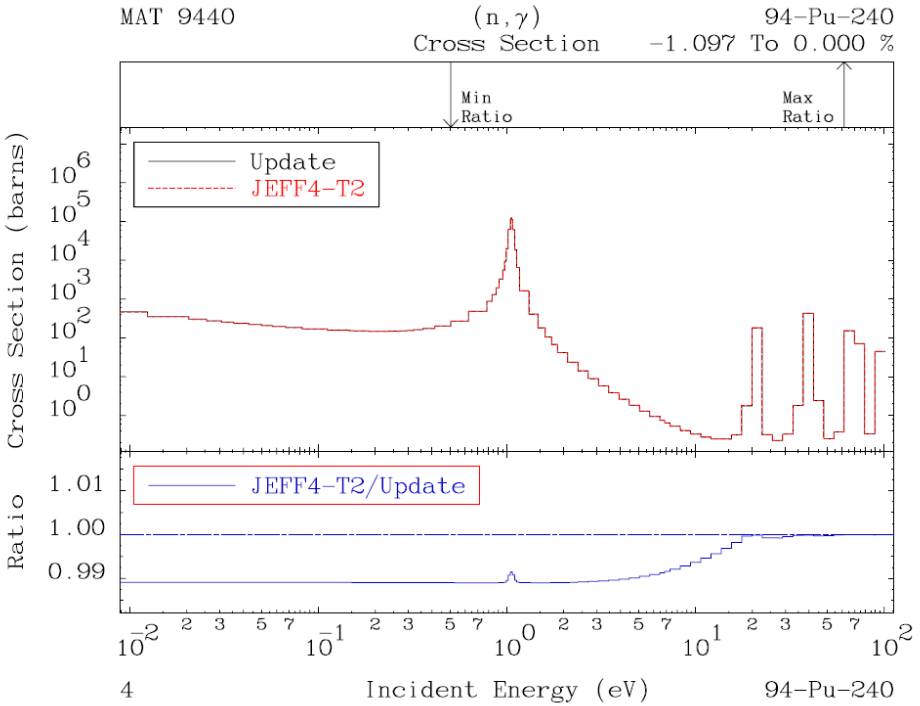
Impact of GLLS on ^{239}Pu(n,g) cross section



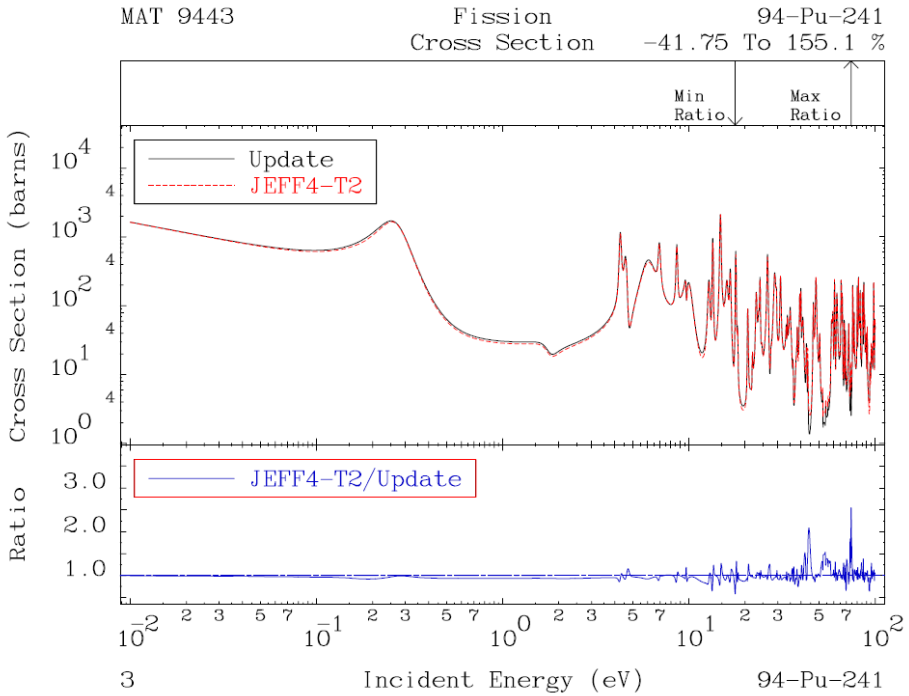


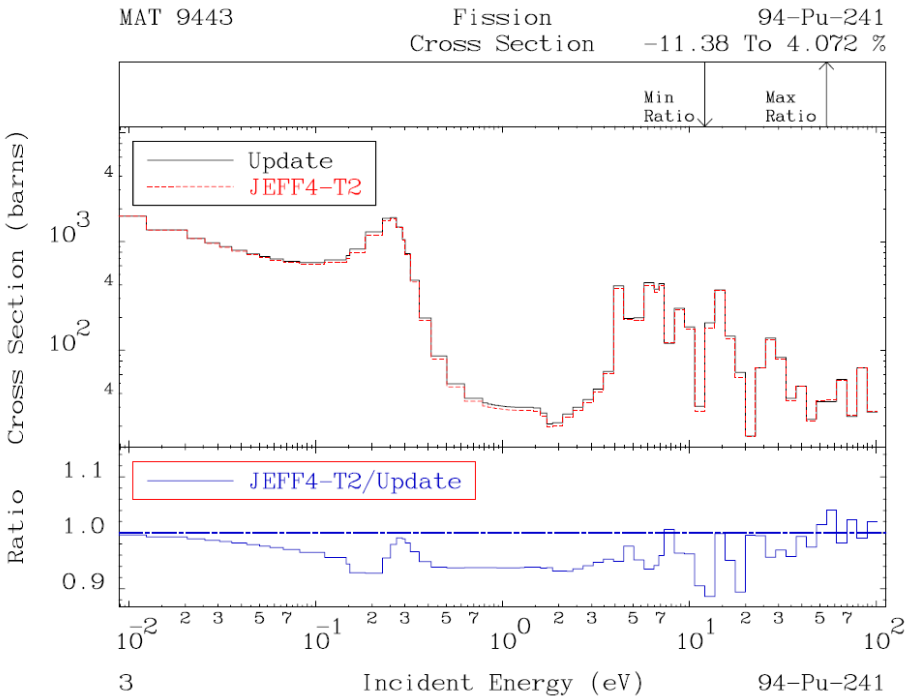
Impact of GLLS on ^{240}Pu(n,g) cross section



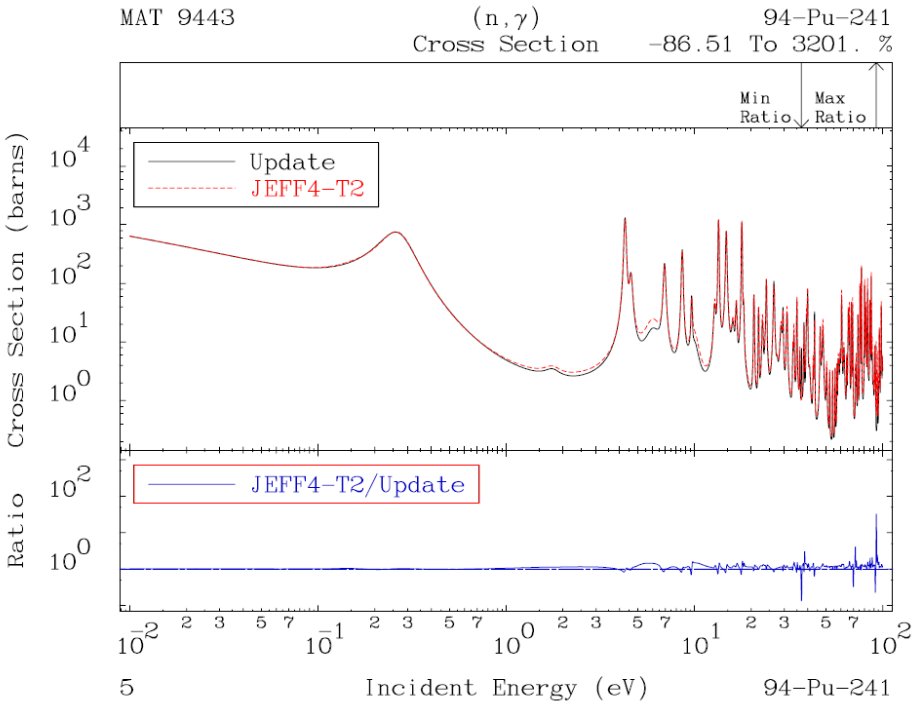


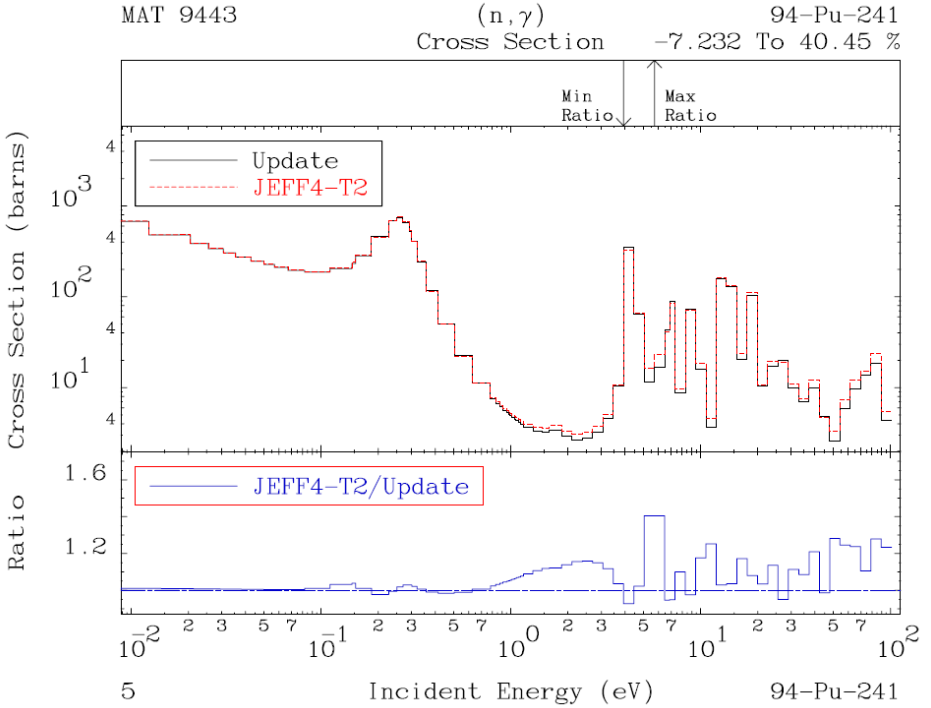
Impact of GLLS on ^{241}Pu(n,f) cross section





Impact of GLLS on ^{241}Pu(n,g) cross section





Verification

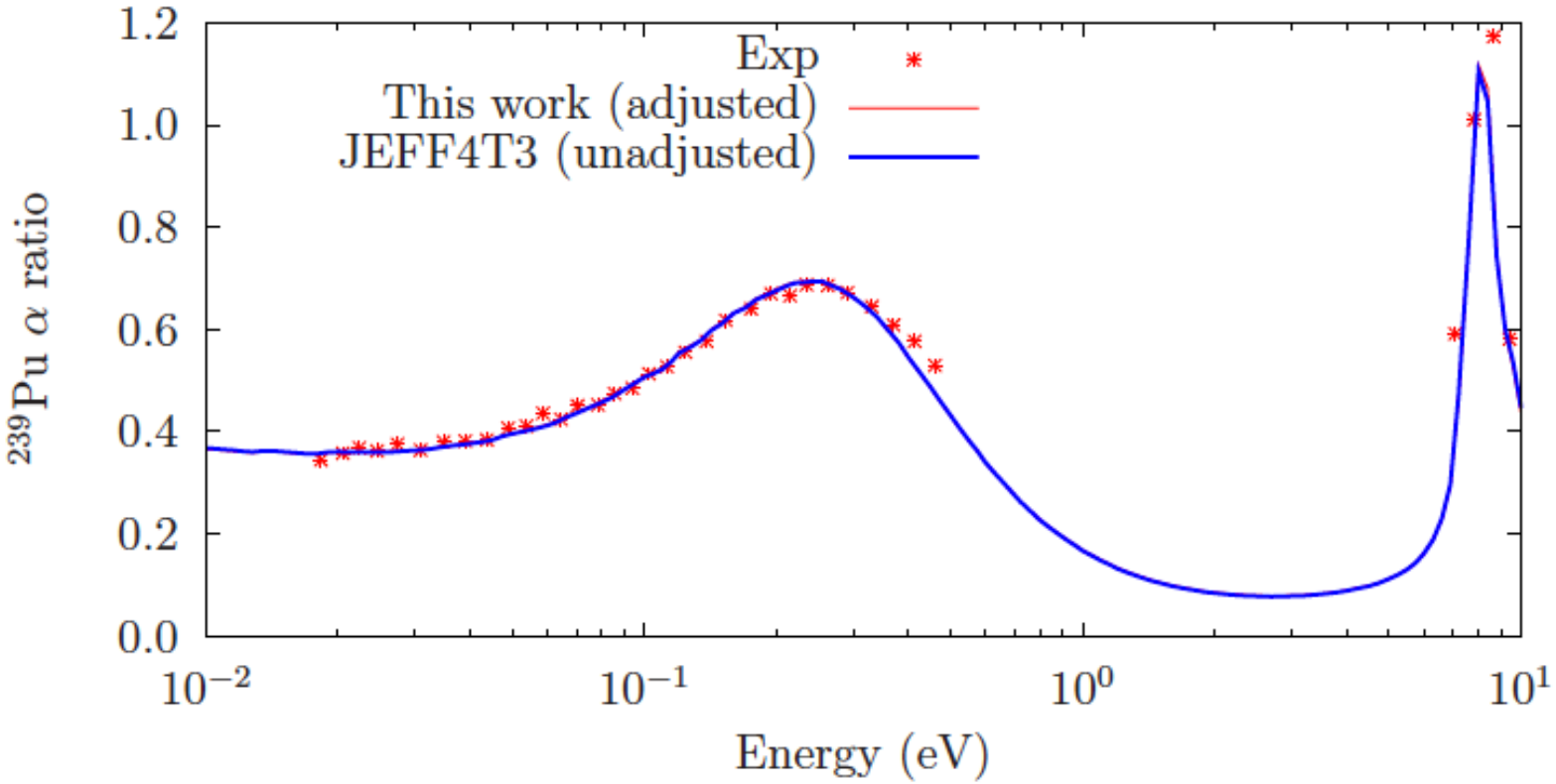
Impact on thermal standards

Table 1: Thermal standard values (Nuclear Data Sheets 148 (2018) 143)

	^{239}Pu(n_{th},f)	^{239}Pu(n_{th},γ)	^{239}Pu $\bar{\nu}_{tot}$	^{241}Pu(n_{th},f)	^{241}Pu(n_{th},γ)	^{241}Pu $\bar{\nu}_{tot}$
Standard	752.4 ± 2.2 b.	269.8 ± 2.7 b.	2.878 ± 0.013	1023.6 ± 10.8 b.	362.3 ± 6.1 b.	2.940 ± 0.013
JEFF-3.1.1	750.1 (-2.3) b.	273.9 (+4.1) b.	2.874 (-0.004)	1012.8 (-10.8) b.	363.2 (-0.1) b.	2.931 (-0.009)
JEFF-3.3	752.7 (+0.3) b.	272.5 (+2.7) b.	2.866 (-0.012)	1012.8 (-10.8) b.	363.2 (-0.1) b.	2.957 (+0.017)
JEFF-4.0T1	749.8 (-2.6) b.	271.0 (+1.2) b.	2.866 (-0.012)	1012.8 (-10.8) b.	363.3 (+0.0) b.	2.947 (+0.007)
JEFF-4.0T2	753.4 (+1.0) b.	269.6 (-0.2) b.	2.879 (+0.001)	1012.8 (-10.8) b.	363.3 (+0.0) b.	2.947 (+0.007)
JEFF-4.0T3(a)	753.0 (+0.6) b.	270.8 (+1.0) b.	2.879 (+0.001)	1025.9 (+2.3) b.	361.1 (-1.2) b.	2.941 (+0.001)
JEFF-4-0T3(u)	751.7 (-0.7) b.	270.2 (+0.4) b.	2.867 (-0.011)	1012.8 (-10.8) b.	363.3 (+0.0) b.	2.947 (+0.007)

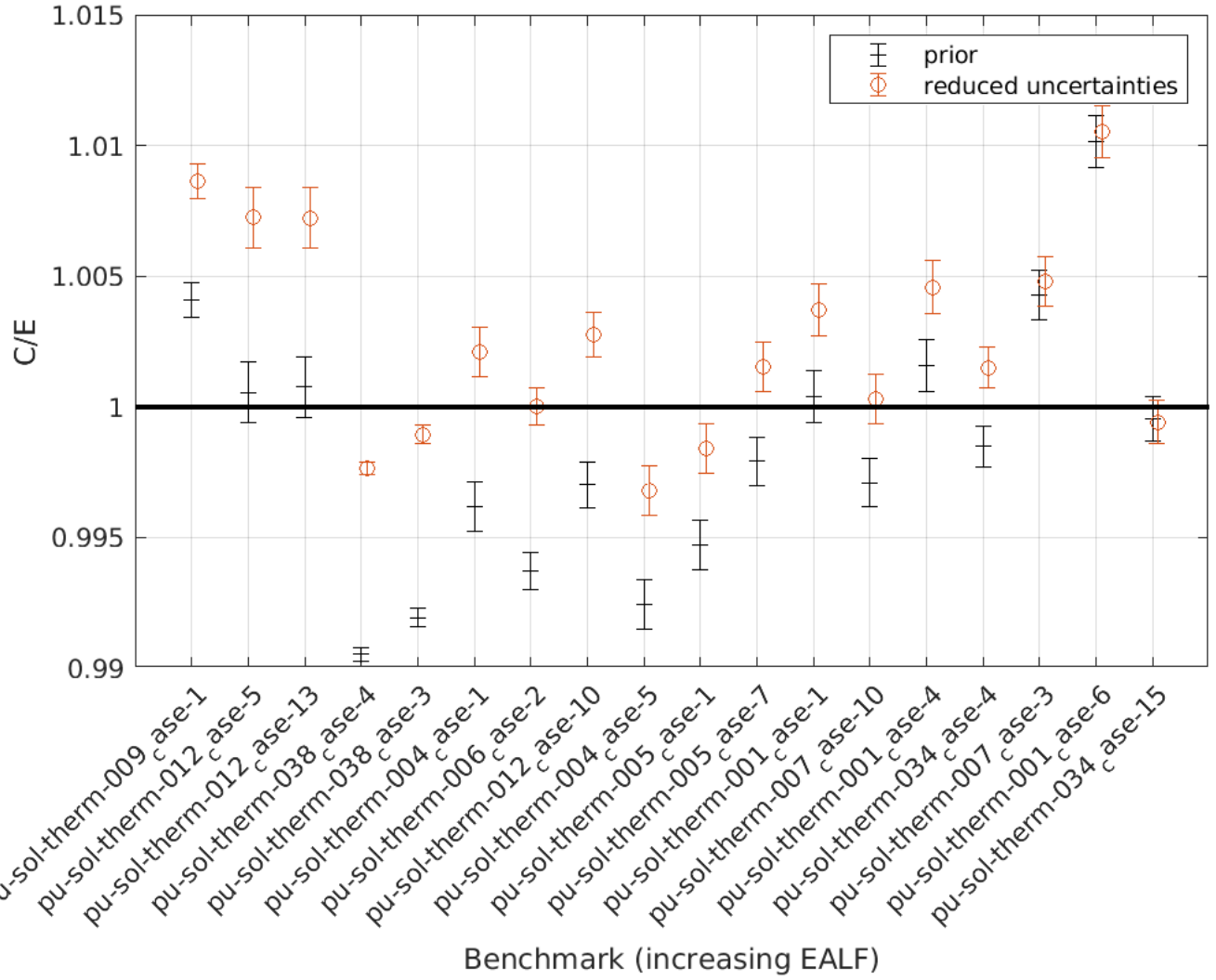
- In JEFF4T3, there are two Pu239 files: one adjusted (this work) and one not adjusted
- Same for Pu240 and Pu241

Impact of GLLS on ^{239}Pu alpha



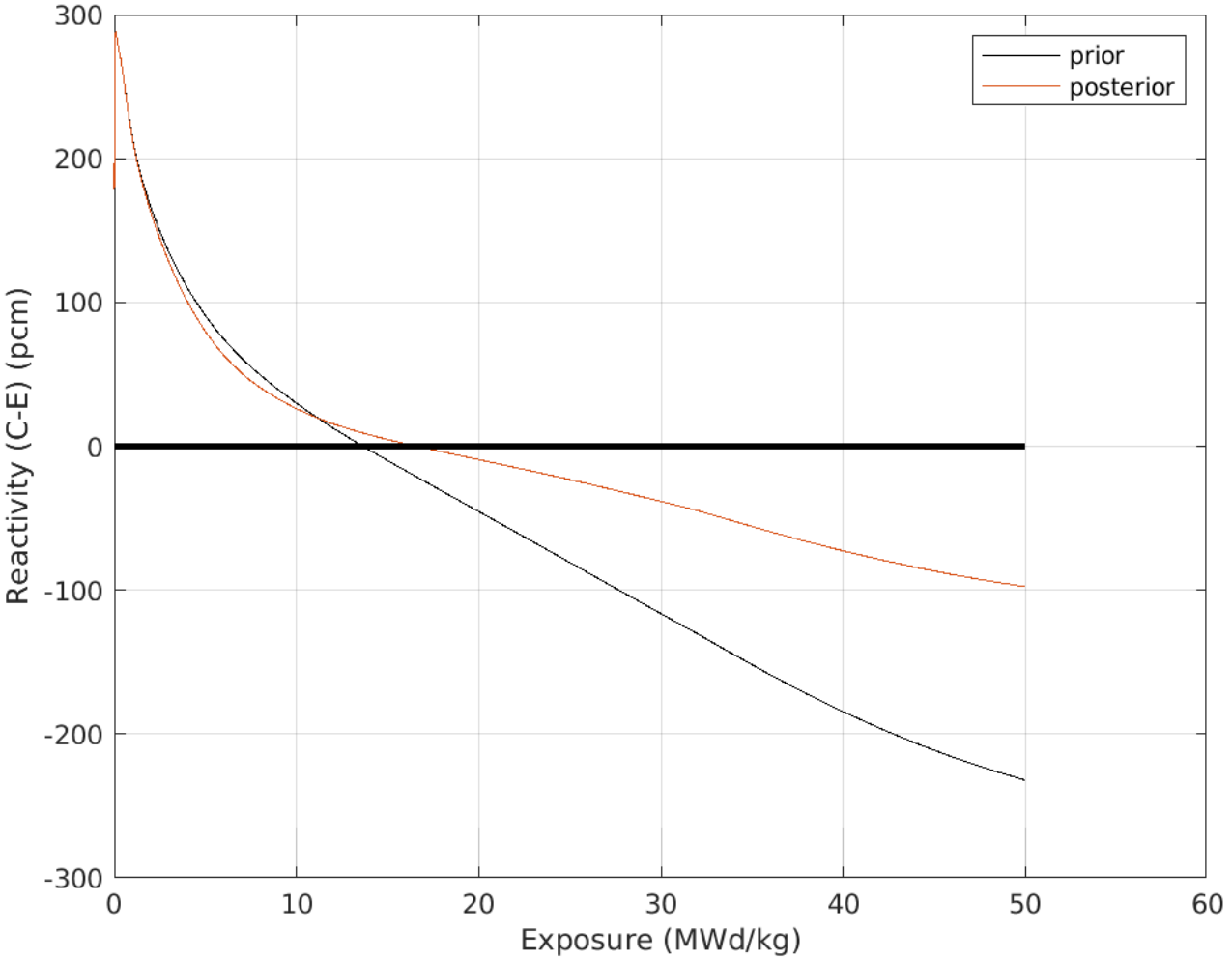
- No noticeable difference

Impact of GLLS on PST benchmarks



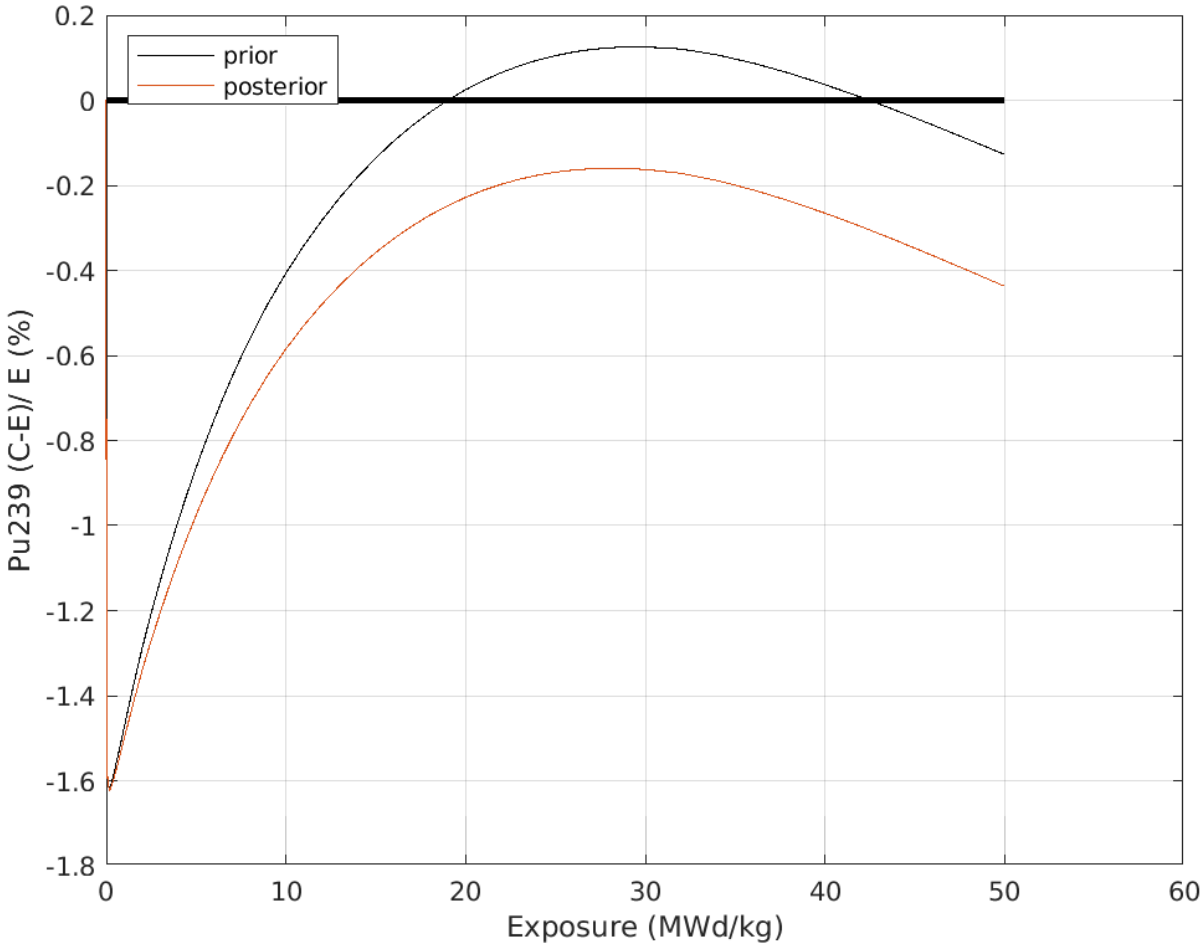
VERA pincell reactivity curve

- Difference with JEFF-3.1.1



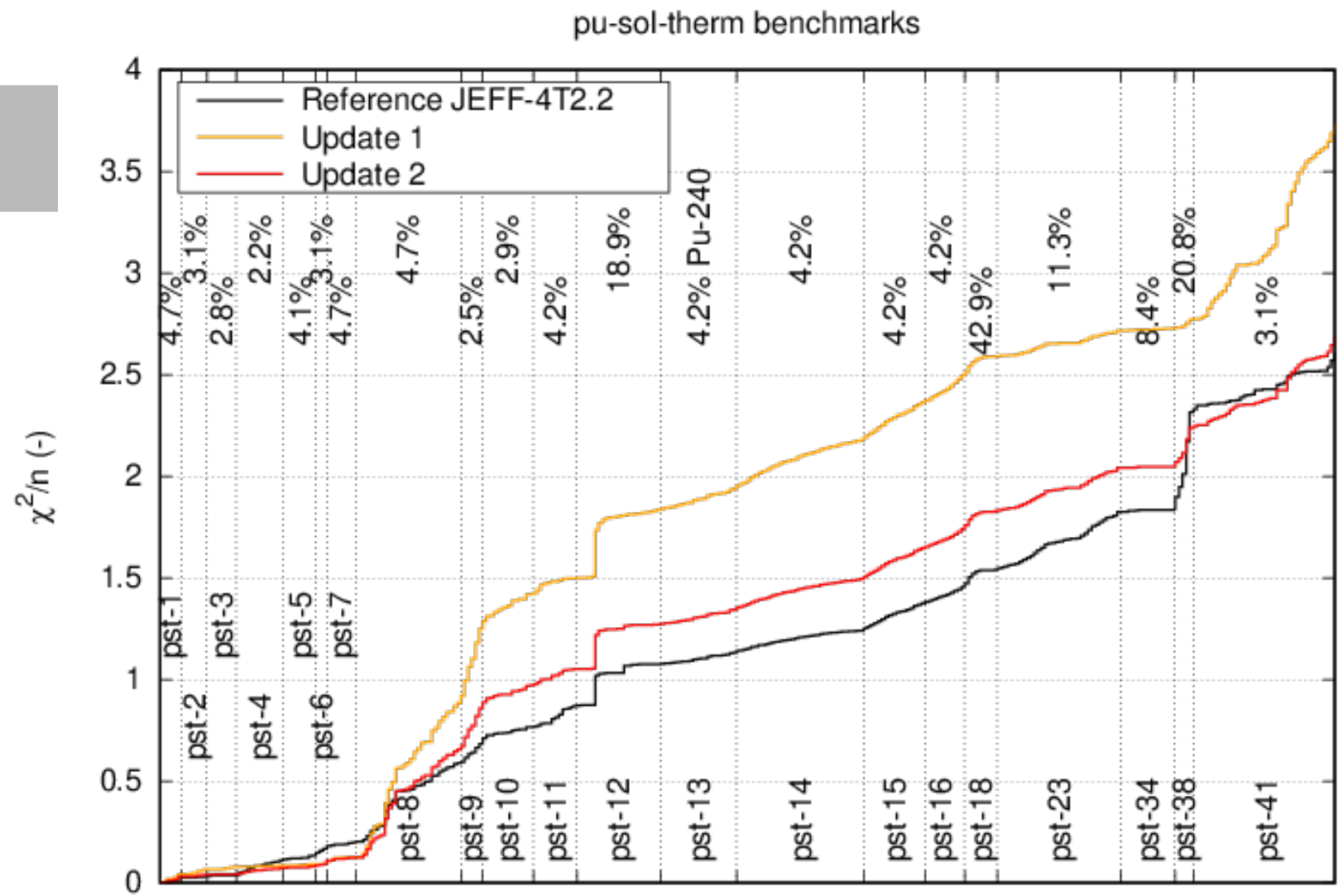
VERA pincell ^{239}Pu build-up

- Difference with JEFF-3.1.1

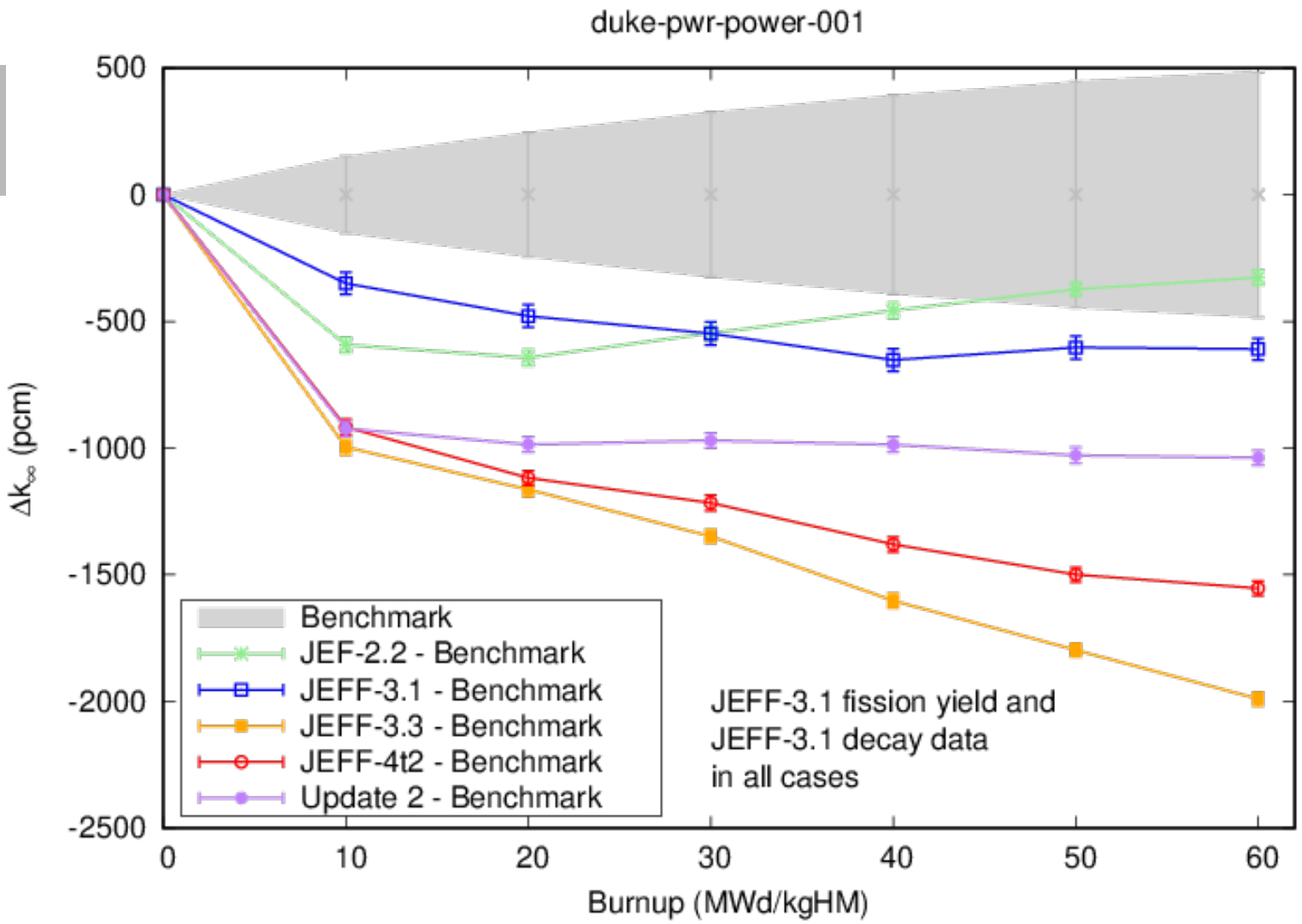


Validation

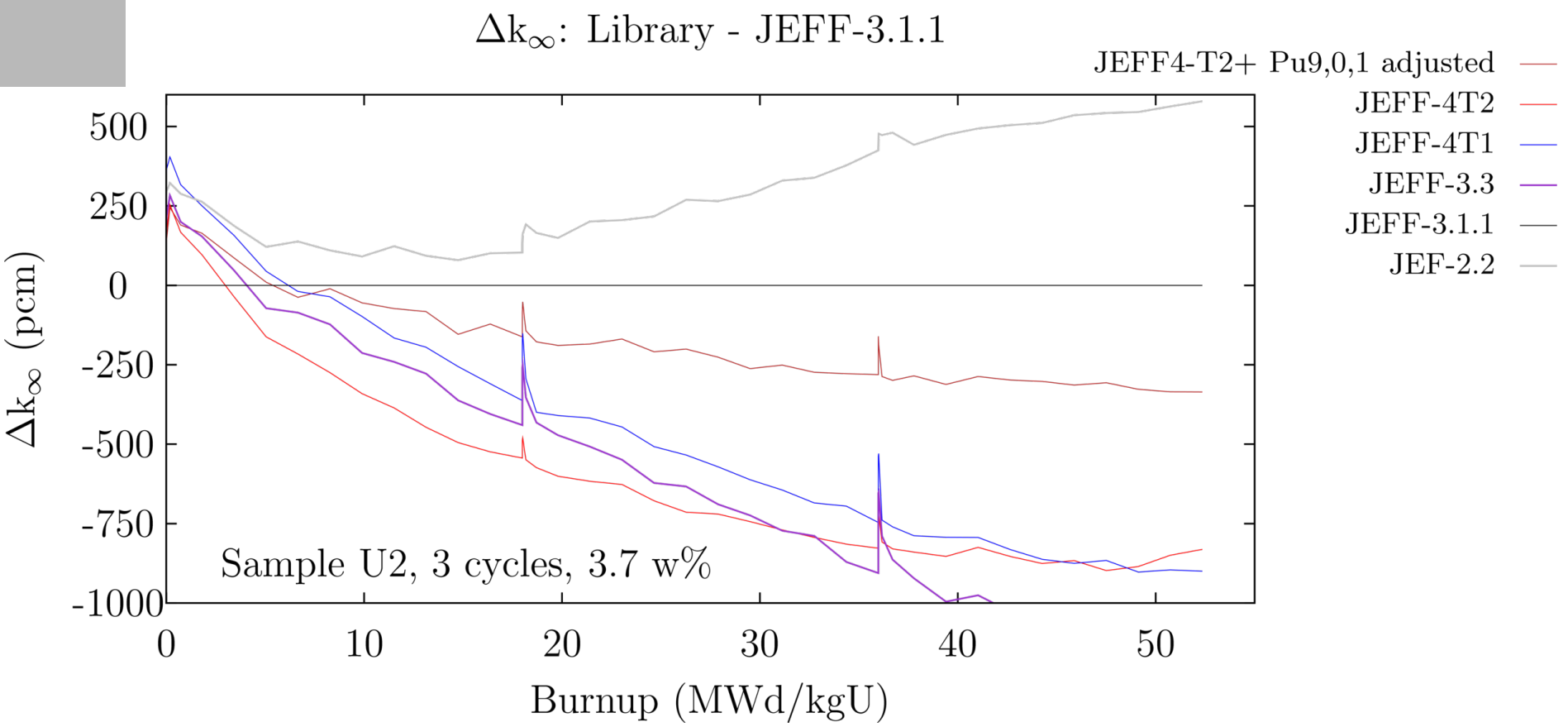
Validation on PST benchmarks (Update 2)



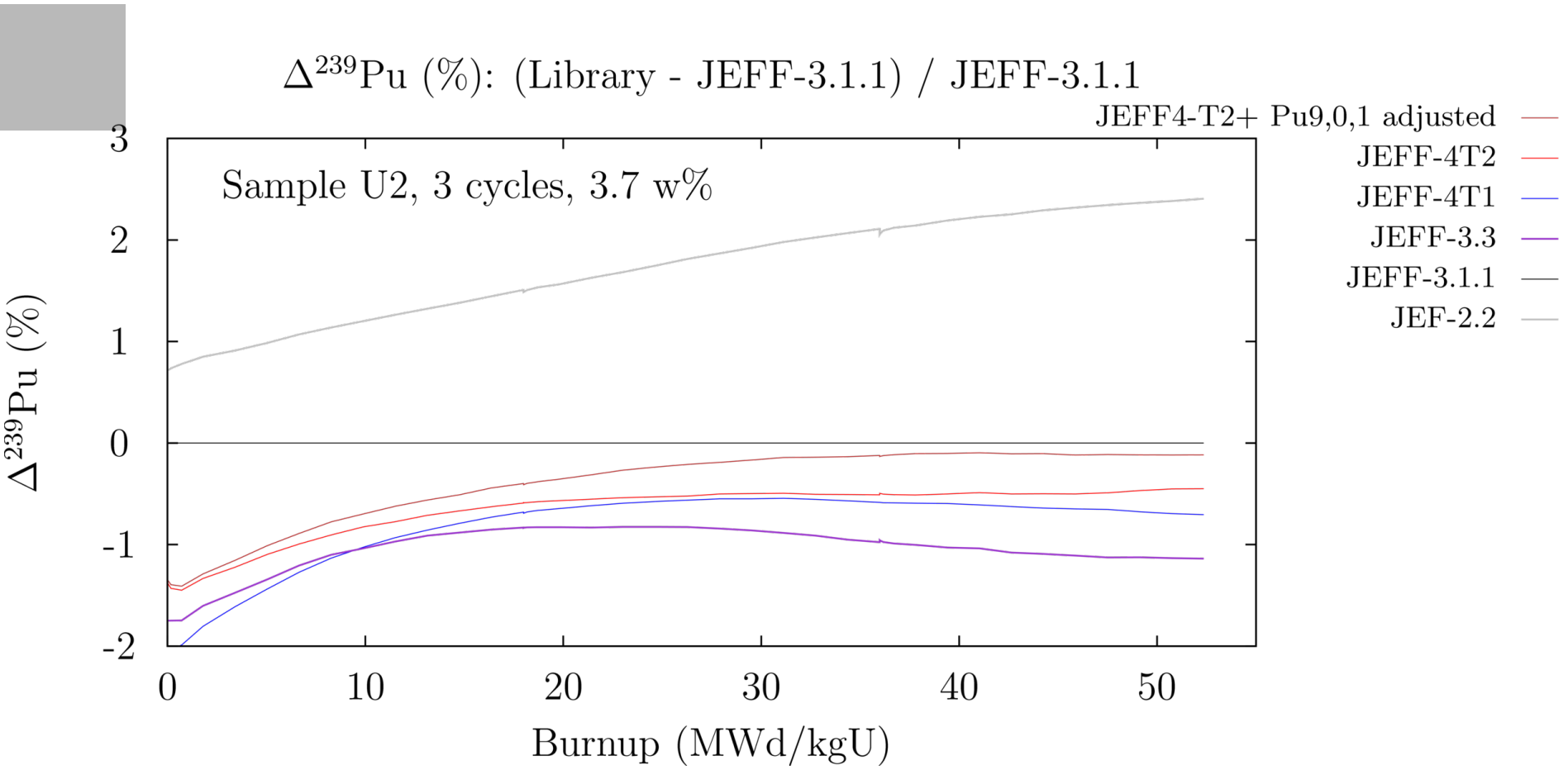
Validation on the Duke PWR benchmark



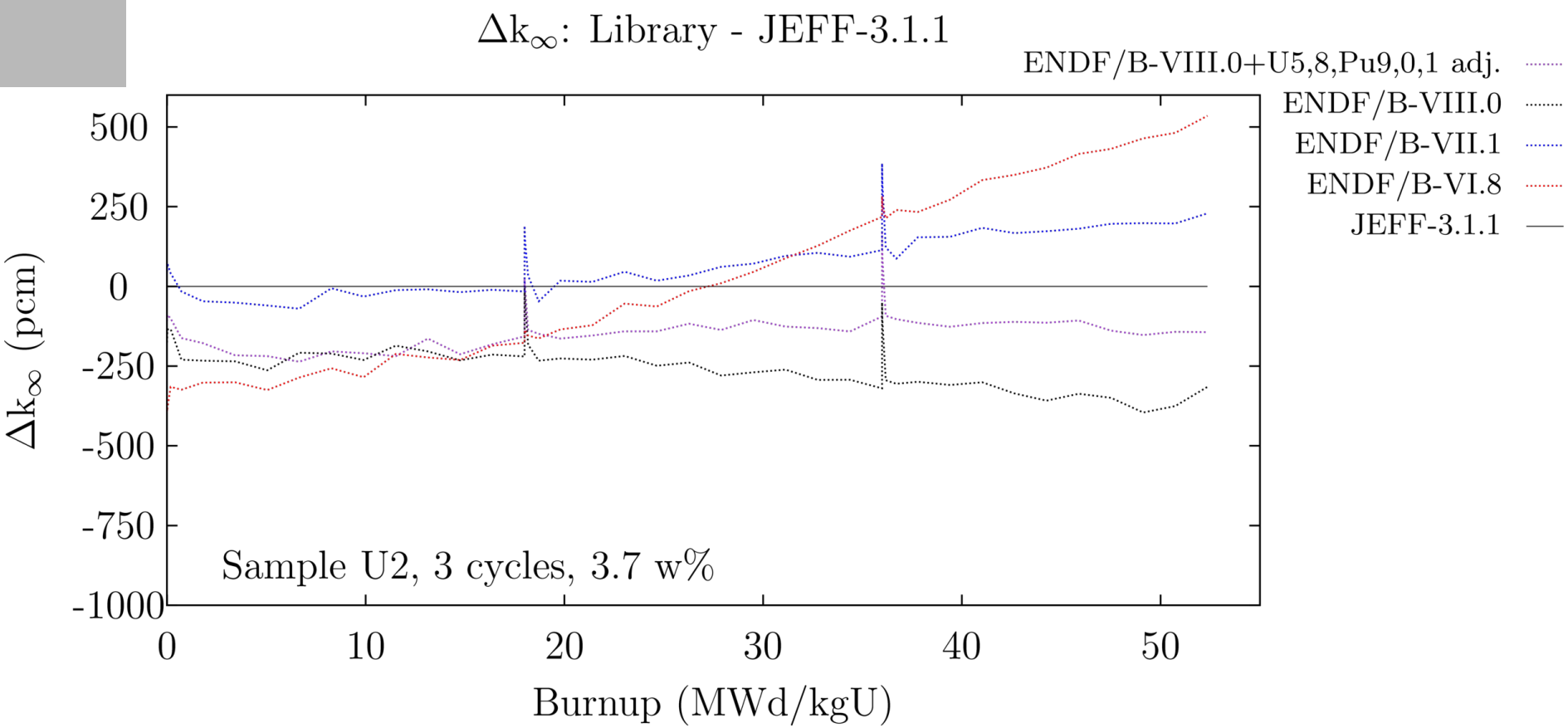
Reactivity with the U2 sample (UO_2)



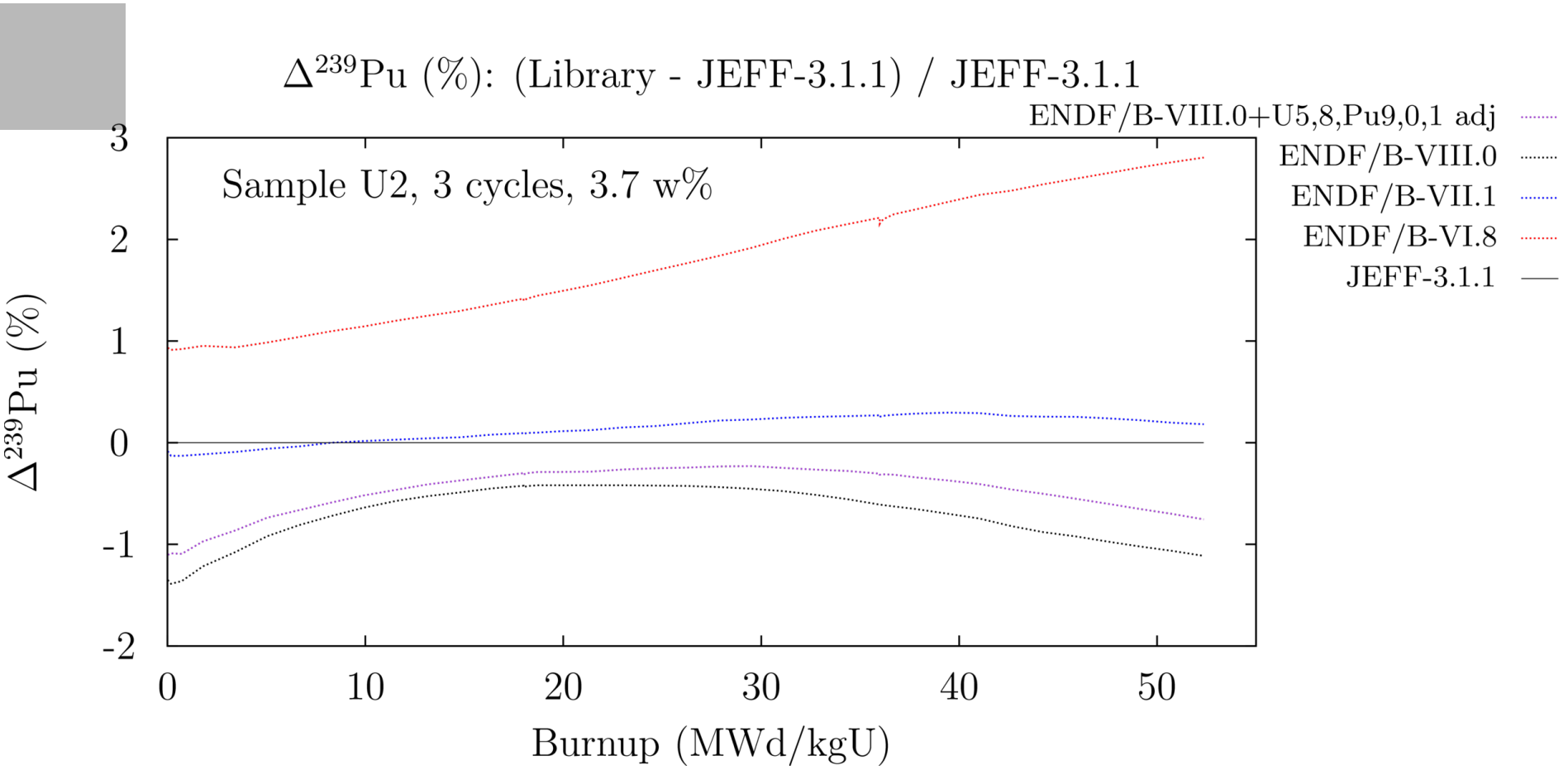
^{239}Pu concentration with the U2 sample (UO_2)



Reactivity with the U2 sample (UO_2)

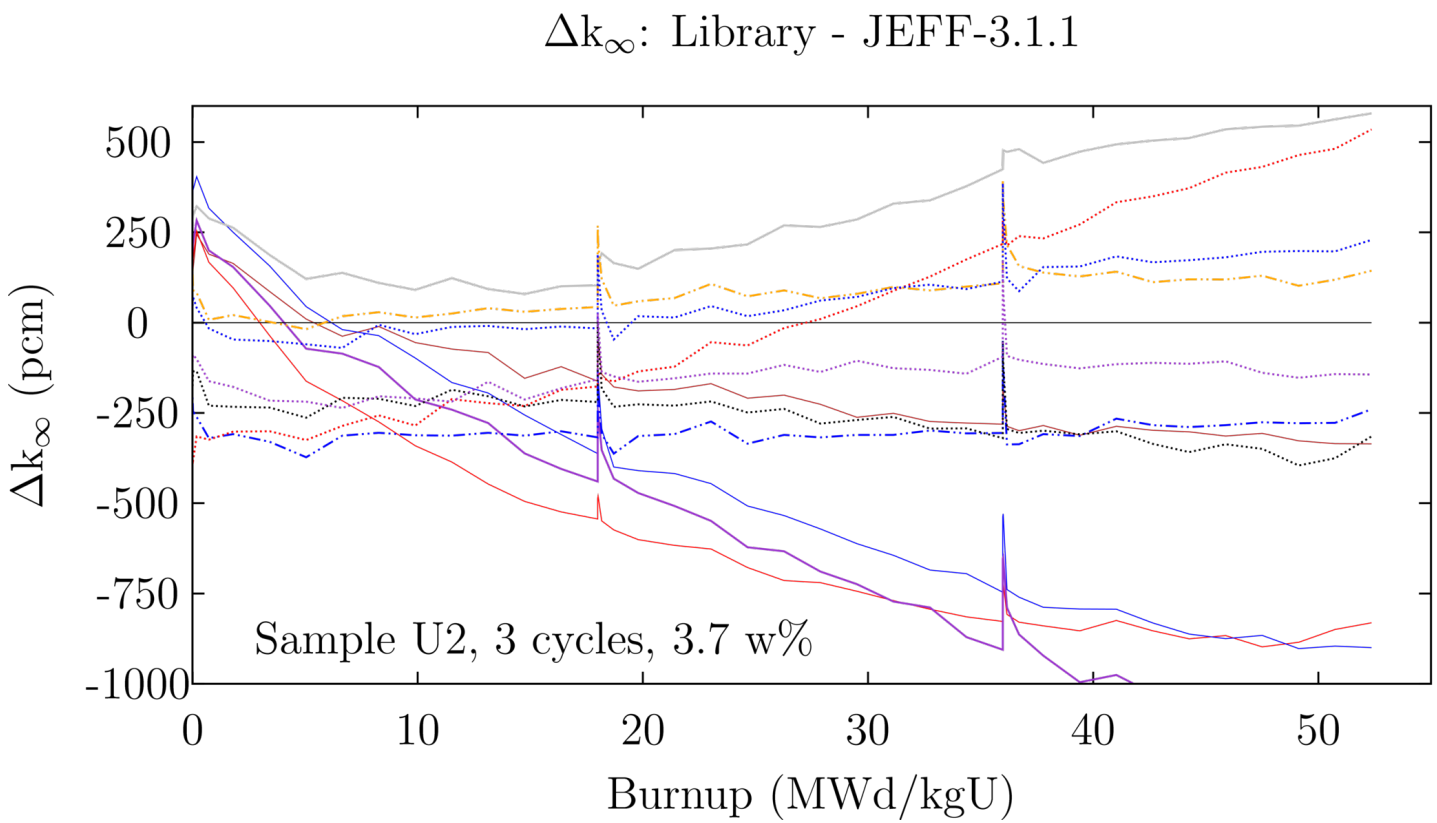


^{239}Pu concentration with the U2 sample (UO_2)

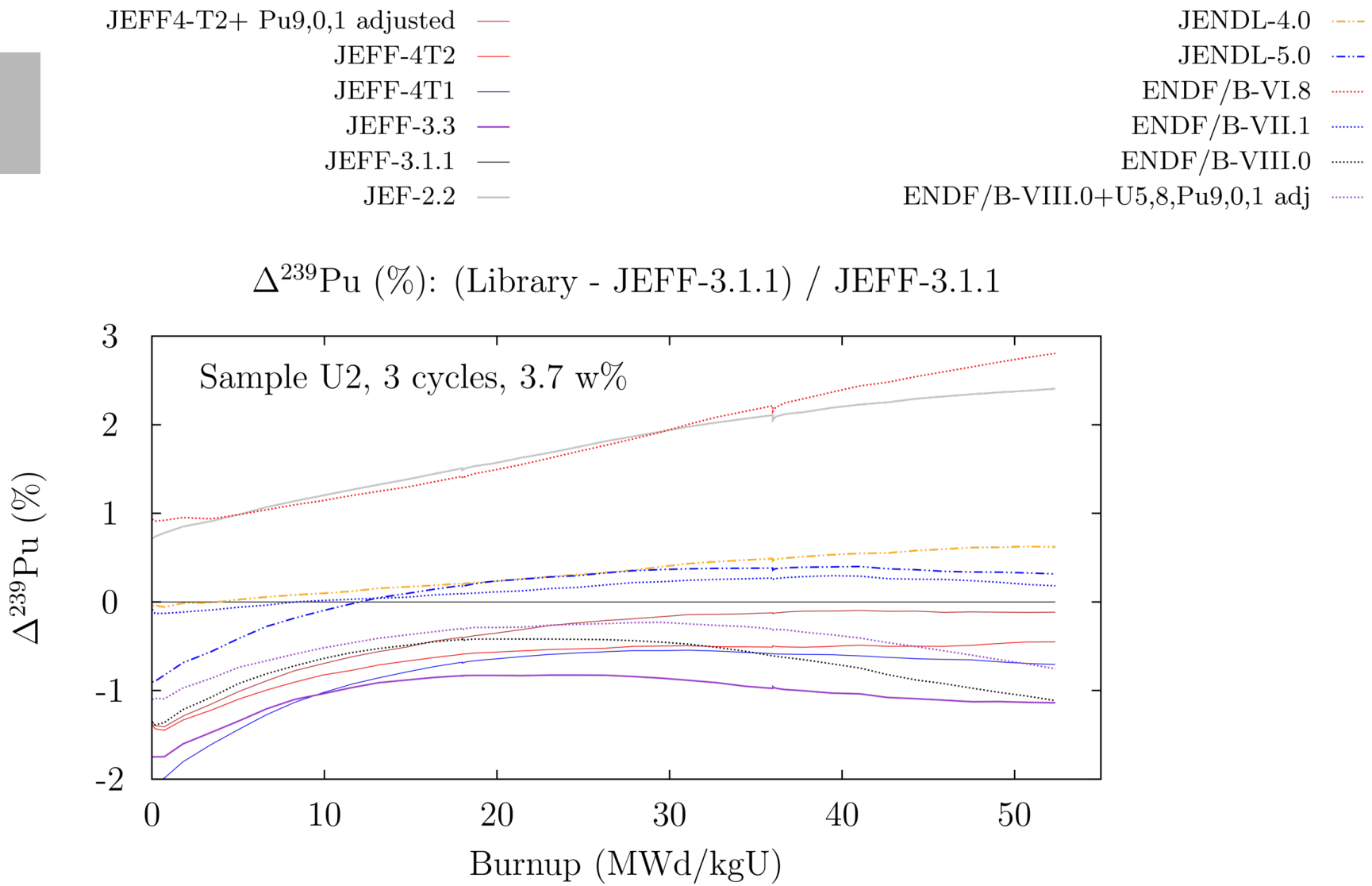


Reactivity with the U2 sample (UO_2)

JEFF4-T2+ Pu9,0,1 adjusted
JEFF-4T2
JEFF-4T1
JEFF-3.3
JEFF-3.1.1
JEF-2.2
JENDL-4.0
JENDL-5.0
ENDF/B-VI.8
ENDF/B-VII.1
ENDF/B-VIII.0
ENDF/B-VIII.0+U5,8,Pu9,0,1 adj.

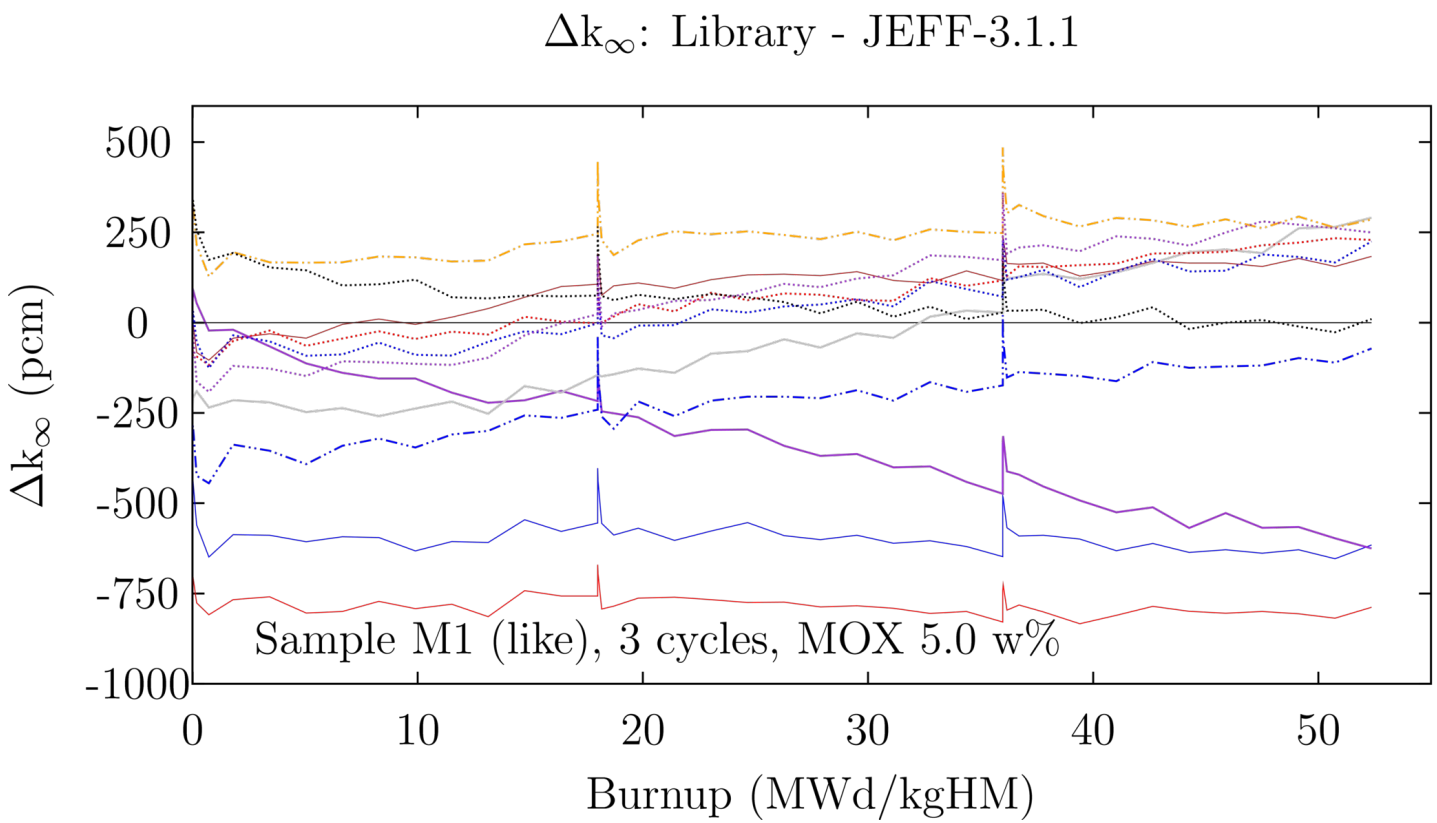


^{239}Pu concentration with the U2 sample (UO_2)



Reactivity with the M1-like sample (MOX)

JEFF4-T2+ Pu9,0,1 adjusted
JEFF-4T2
JEFF-4T1
JEFF-3.3
JEFF-3.1.1
JEF-2.2
JENDL-4.0
JENDL-5.0
ENDF/B-VI.8
ENDF/B-VII.1
ENDF/B-VIII.0
ENDF/B-VIII.0+U5,8,Pu9,0,1 adj.



Conclusion

- New adjusted ^{239,240,241}Pu (NRG, EPFL, PSI)
  - Perform as expected with JEFF-4T2 (note that ^{238}U was already adjusted in JEFF-4T2)
  - Proposed for JEFF-4T3

- What's next in JEFF:
  - Adjusting solely Pu isotopes is not enough
  - Plans for a complete adjustment with U and Pu (not yet approved)

- Test on new adjusted ^{235,238}U, ^{239,240,241}Pu from ENDF/B-VIII.1beta (IAEA) indicates good performances on UO_2 and MOX samples

Slides from Mathieu

- Dear colleagues,
- We have adjusted the 3 isotopes Pu239, 240 and 241, in order to improve the burnup dependence and some other issues related to JEFF-4.0T2.
- You can find the updated files here:
-
- -Pu239: https://tendl.web.psi.ch/tendl_2021/tar_files/94-pu-239g_may2023_1.1_pfns_j33.update2
- -Pu240: https://tendl.web.psi.ch/tendl_2021/tar_files/94-pu-240g.update2
- -Pu241: https://tendl.web.psi.ch/tendl_2021/tar_files/94-pu-241g_may2023_0.update2
-
- Some descriptive text is given in the MF1 of the above files. A bit in details, here is our approach:
- For burnup and k_inf, match the result of JEFF-3.1.1, based on a PWR pincell calculation (3.1%)
- For burnup and Pu239 concentration (at the end of irradiation), be close to the JEFF-3.1.1 performances
- For thermal standard values, stay close to (n,f) and (n,g) for Pu239 and Pu241
- Keep the evaluated alpha value close to exfor
- Improve 18 PSTs and 2 kritz
-
- The method is plain GLLS updates for resonance parameters (for the 3 isotopes) and nubar (for Pu239).
- You can see some results of our pre-benchmarking below. The quality of the plots are not always the best, but it gives a good idea.
- We are proposing these files for JEFF-4.0T3, but we would appreciate your feedback before the files are included in the T3 distribution.
- Any remark is welcome, and we are ready to update the work if necessary.
-
- Best Regards,
- Dimitri, Mathieu and Steven

Guiding RRR parameters of Pu-239,240 & 241

- Modification of the Γ_n Γ_g Γ_{f1} and Γ_{f2} for the first 24 resonances of Pu-239, first 9 resonances of Pu-240 and first 47 resonances of Pu-241 one at a time to determine sensitivity coefficients with Dragon

- Production of a variance matrix for the 325 input parameters
  - All width have a uncertainty of 1%; no correlation with other parameters
  - Nubar below 16eV (14 groups) with an uncertainty of 0.1% and no correlations

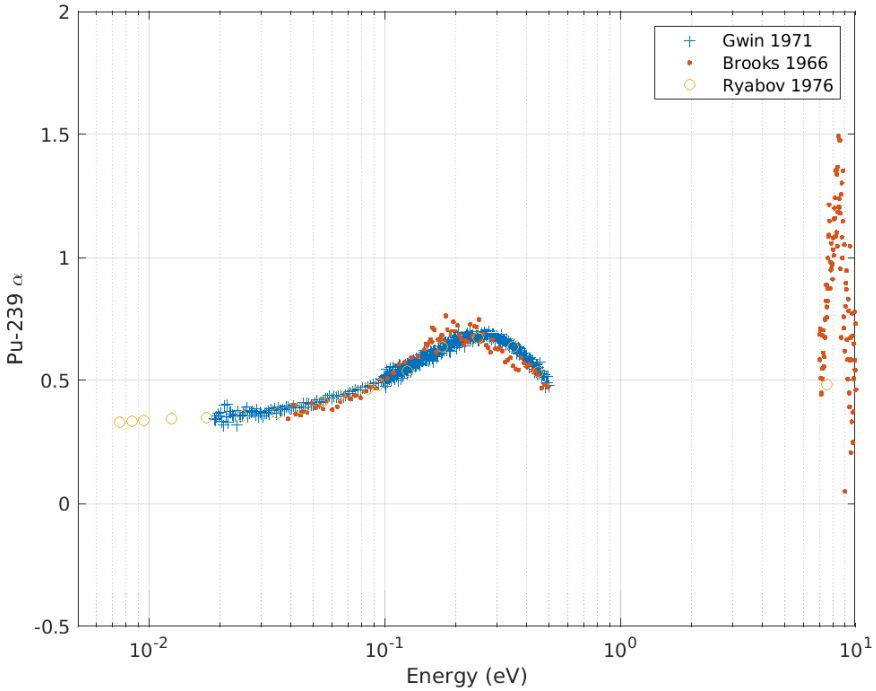
- Bayesian inference using GLLS and a number of “experimental” constraints (see next slide)

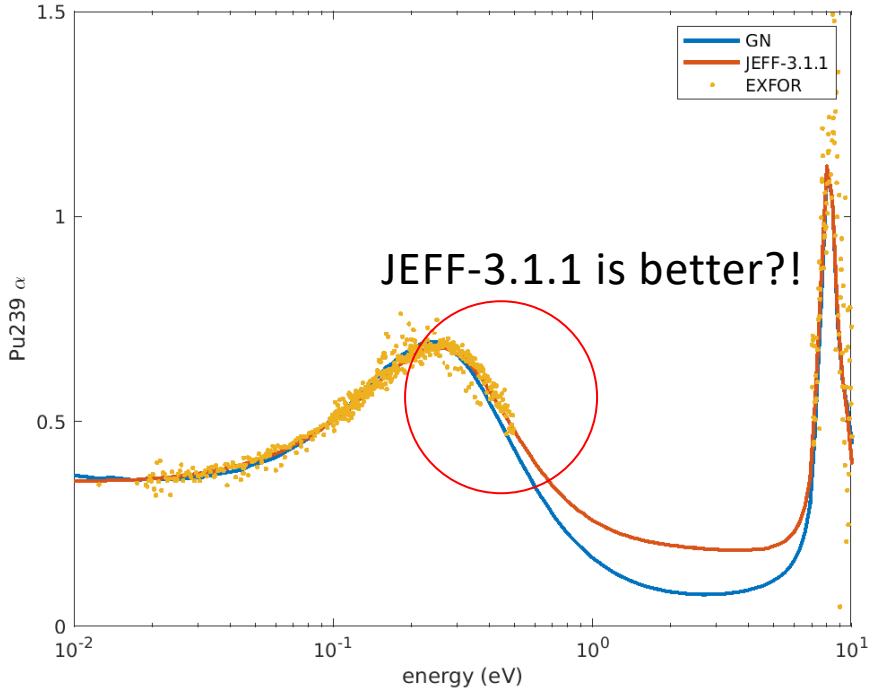
“Experimental data” used in the Bayesian inference exercise

1. Matching the Jeff-3.1.1 pincell results (!)
   - K-inf with an uncertainty of 100pcm (56 points)
   - Pu-239 concentration with an uncertainty of 1% (55 points)
2. Pu-239,241 thermal capture and fission standards (4 points)
   - https://www-nds.iaea.org/standards/std2017/Standards2017_TNC.txt
3. A number of alpha ratio from EXFOR suggested in jefdoc-2251 (37 points)
   - Brooks 1966
   - Gwin 1971
   - Ryabov 1976
4. 18 PSTs benchmarks and 2 Kritz

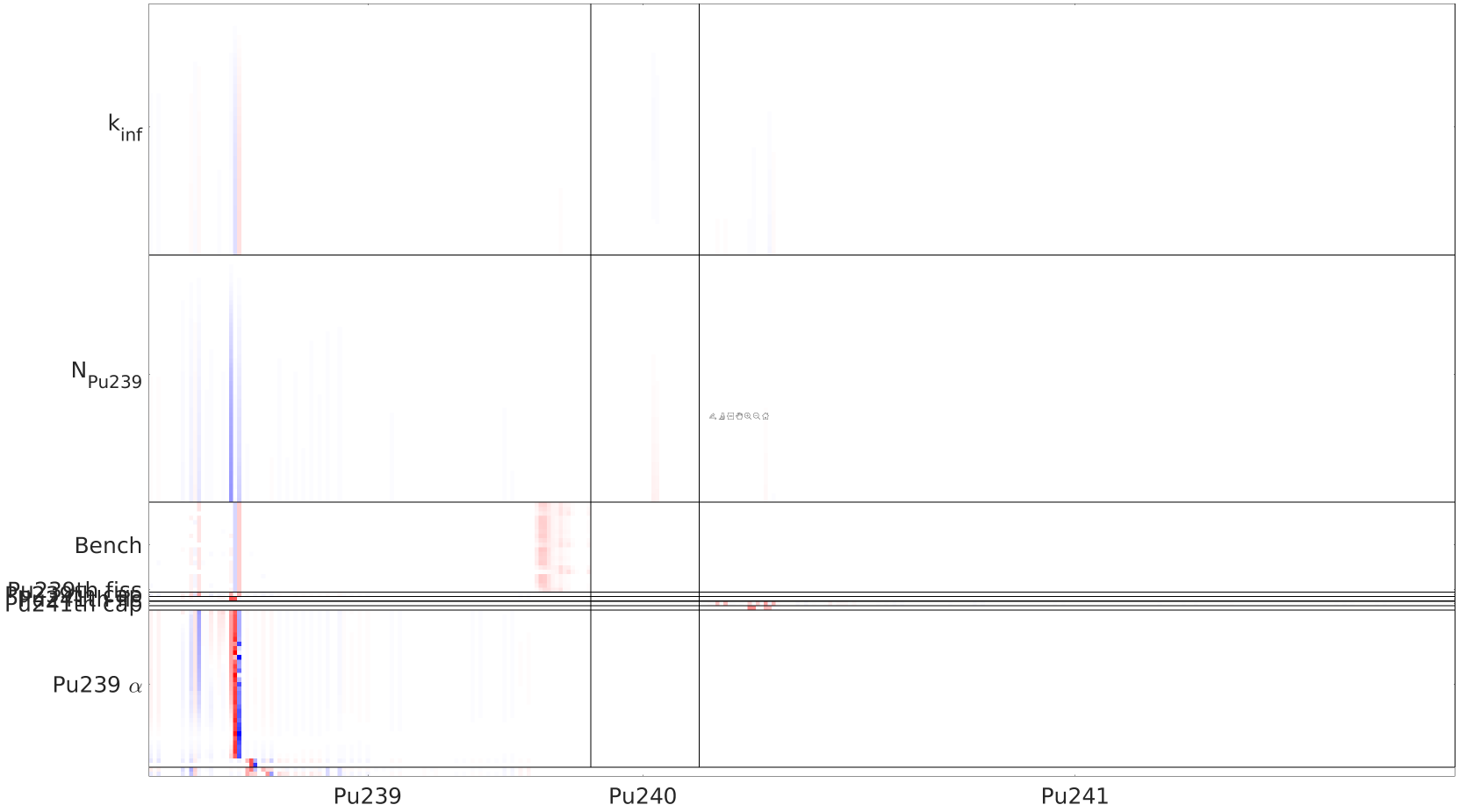
- All “experimental” data points are considered equally important in the exercise
- Benchmarks uncertainties are reduced by a factor 5
- For the alpha value, a naïve approach is taken
  - all the experimental data points falling in a given energy group of the 685g structure is averaged together with its relative uncertainty (no weighting)
  - all the energies between 0.5 and 7 eV are removed (too much jitter and possible contamination)
  - every other energy point is removed

Subset of EXFOR data used for Pu-239 alpha



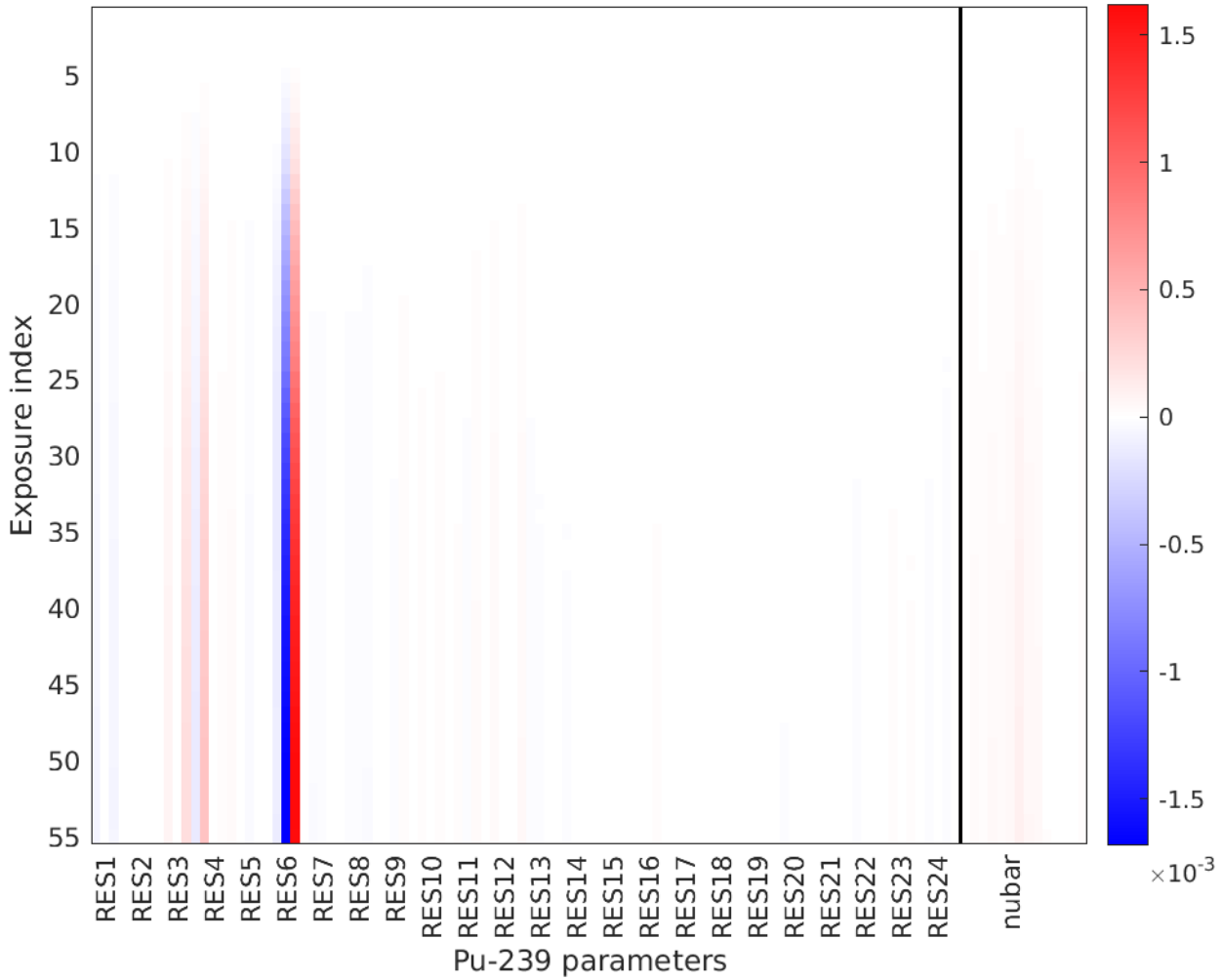


Sensitivties



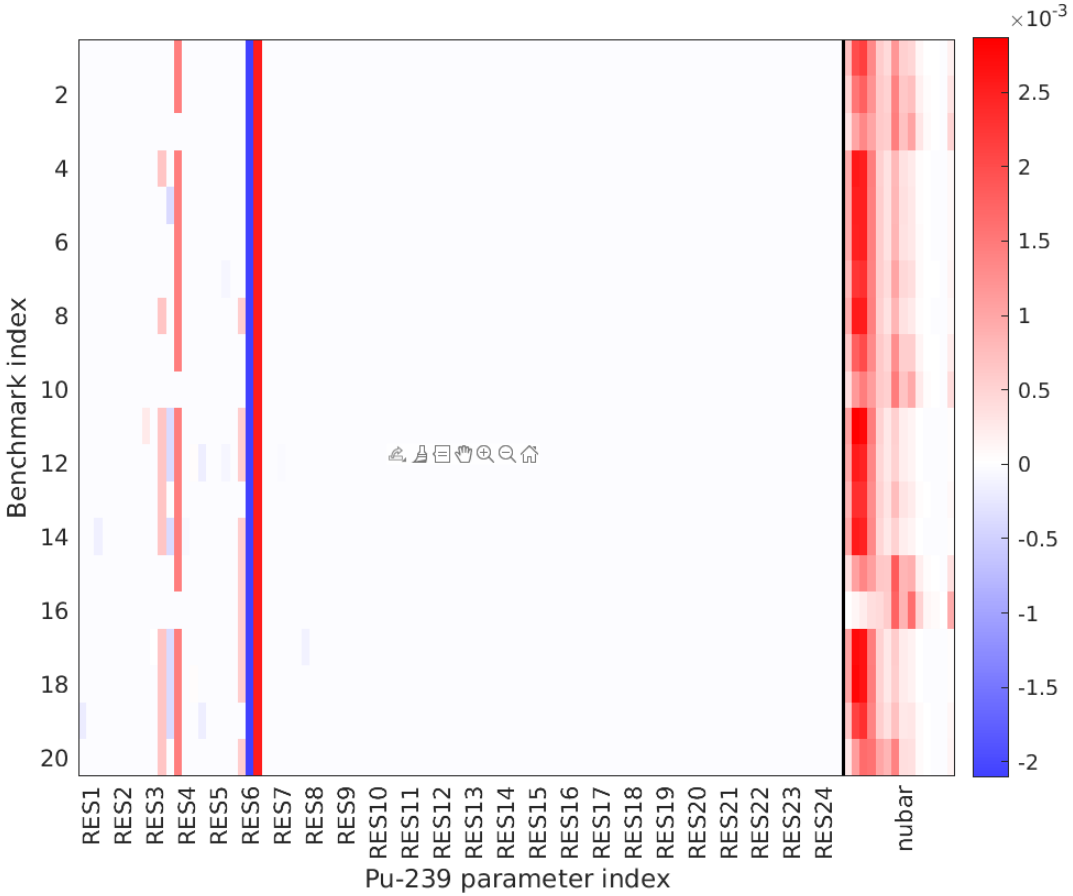
Pincell k-inf sensitivties to Pu-239

- 6th resonance matters most (0.24eV), mainly Gf1 (+) and Gg(-); increasing sensitivity of nubar (+) with exposure less visible due to larger number of groups



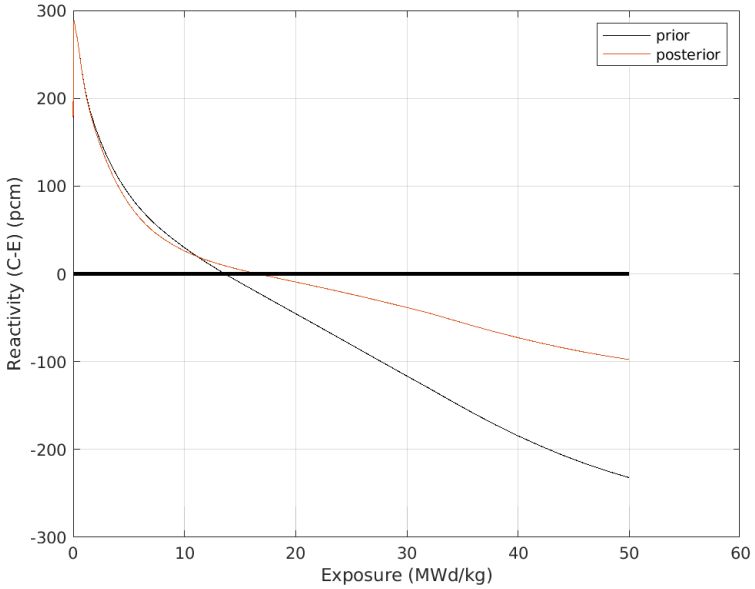
Benchmark sensitivties to Pu-239

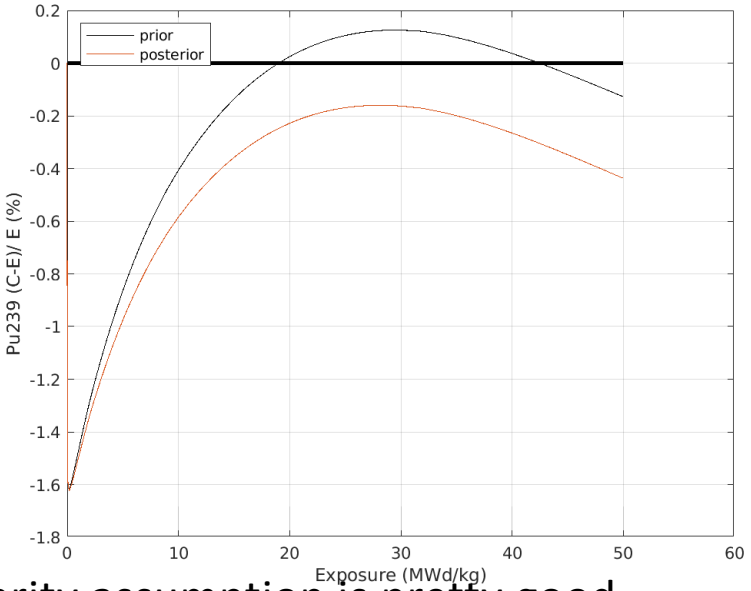
- Benchmark list:
  1. pu-sol-therm-001_case-1
  2. pu-sol-therm-001_case-4
  3. pu-sol-therm-001_case-6
  4. pu-sol-therm-004_case-1
  5. pu-sol-therm-004_case-5
  6. pu-sol-therm-005_case-1
  7. pu-sol-therm-005_case-7
  8. pu-sol-therm-006_case-2
  9. pu-sol-therm-007_case-3
  10. pu-sol-therm-007_case-10
  11. pu-sol-therm-009_case-1
  12. pu-sol-therm-012_case-5
  13. pu-sol-therm-012_case-10
  14. pu-sol-therm-012_case-13
  15. pu-sol-therm-034_case-4
  16. pu-sol-therm-034_case-15
  17. pu-sol-therm-038_case-3
  18. pu-sol-therm-038_case-4
  19. kritz-lwr-resr-001-case-1
  20. kritz-lwr-resr-001-case-2
- Use of ksen for nubar sensitivity



K-inf and Pu-239 concentration

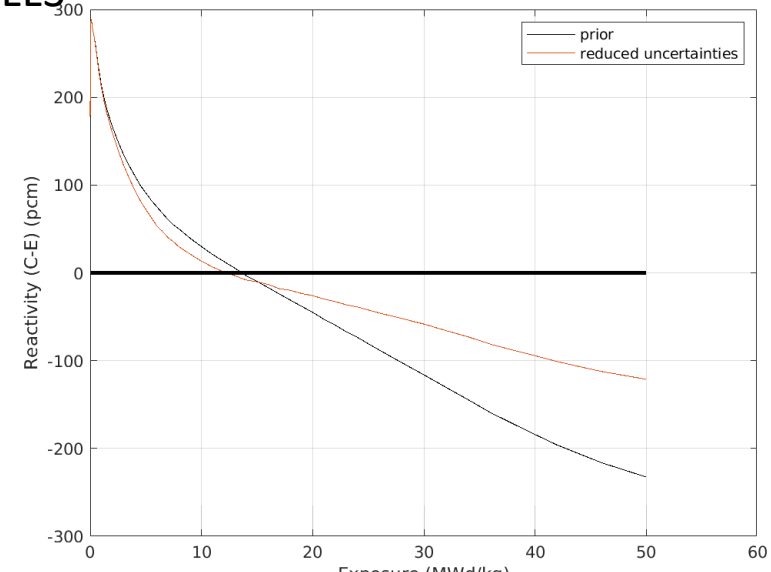
New files

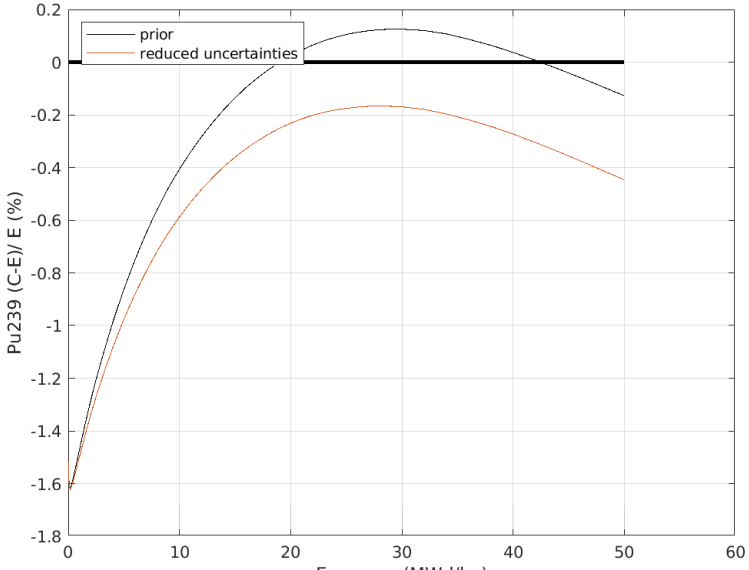




Linearity assumption is pretty good

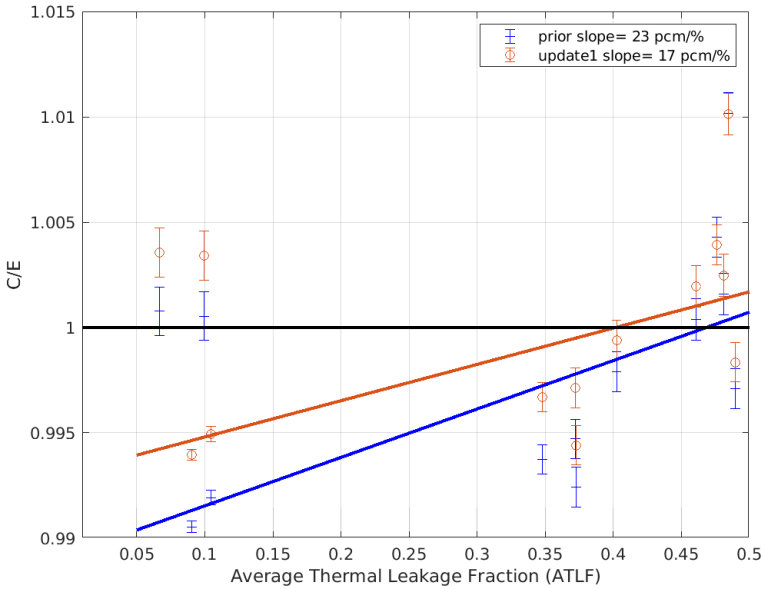
GLLS





Benchmarks

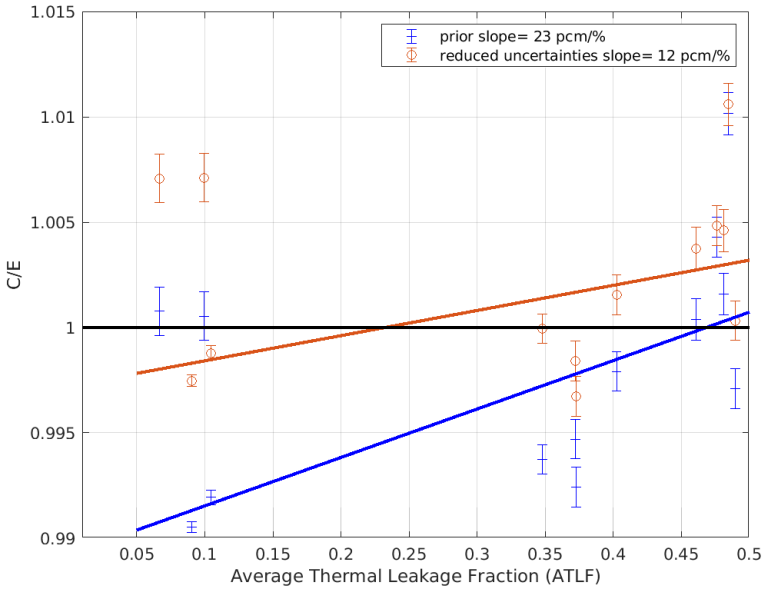
New files



The improvement is not as good

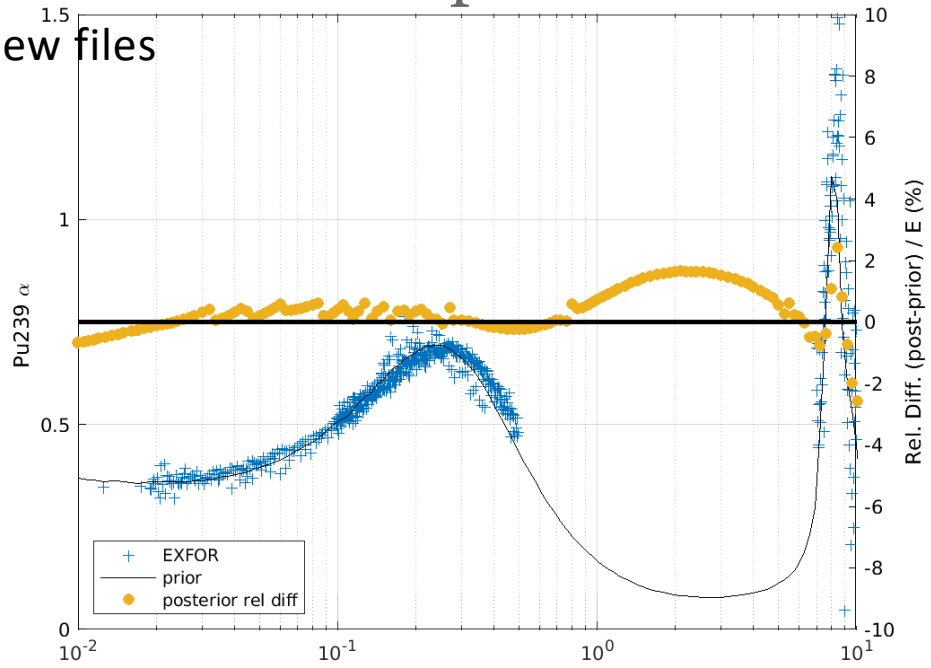
Linearity effect?

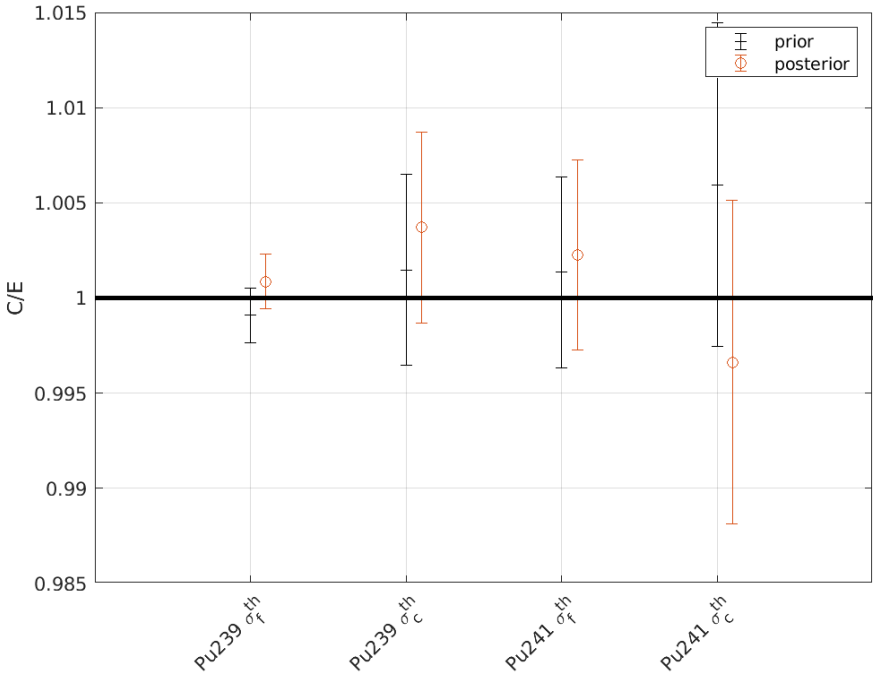
GLLS



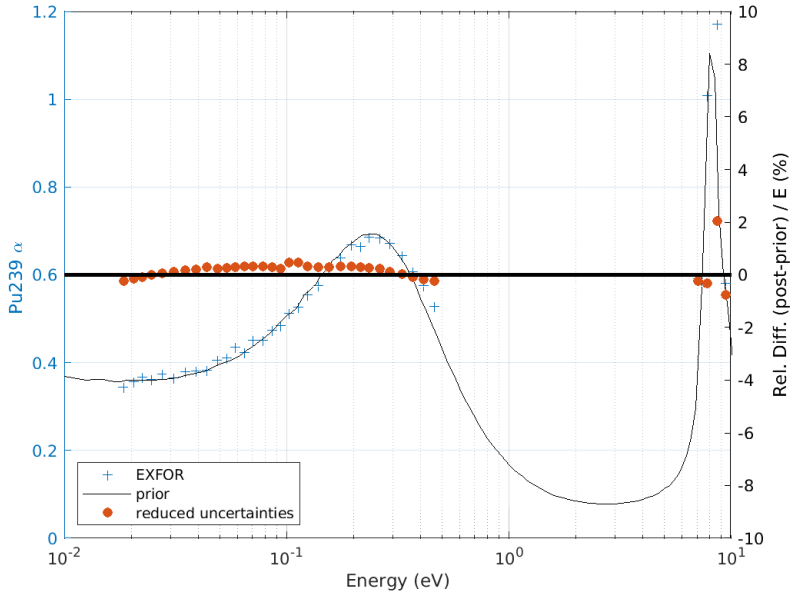
Alpha & standards

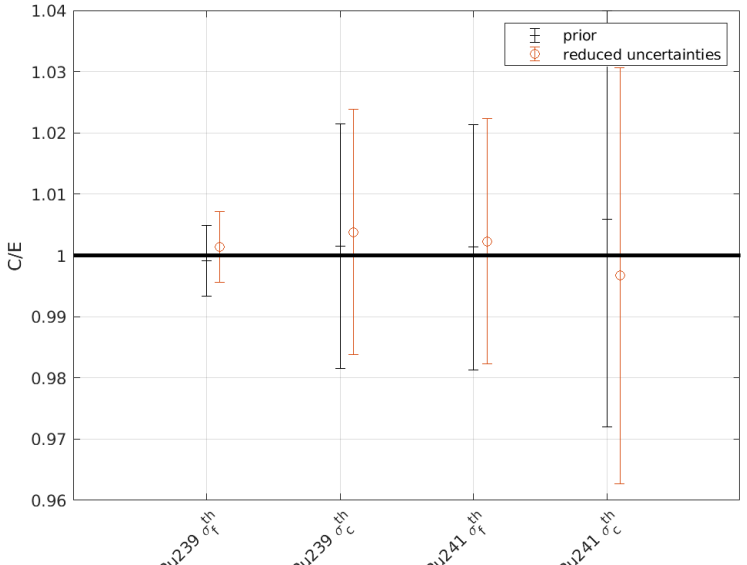
New files





GLLS





Adjusted input parameters

1	P239	-162Gn	0.5%	-3.3%	-2.3%	0.9%
2	P239	-162Gg	0.0%	0.0%	0.1%	0.1%
3	P239	-162Gf1	0.6%	4.0%	6.3%	3.6%
4	P239	-162Gf2	0.0%	0.0%	0.0%	0.0%
5	P239	-8.07Gn	0.0%	0.0%	0.0%	0.0%
6	P239	-8.07Gg	0.0%	0.0%	0.0%	0.0%
7	P239	-8.07Gf1	0.0%	0.0%	0.0%	0.0%
8	P239	-8.07Gf2	0.0%	0.0%	0.0%	0.0%
9	P239	-5.91Gn	-1.0%	-16.5%	-20.5%	-11.1%
10	P239	-5.91Gg	0.0%	0.2%	0.3%	0.2%
11	P239	-5.91Gf1	0.9%	5.2%	4.2%	3.2%
12	P239	-5.91Gf2	-0.2%	-4.0%	-3.3%	-1.6%
13	P239	-0.218Gn	1.9%	4.6%	2.7%	1.5%
14	P239	-0.218Gg	0.0%	1.1%	1.3%	0.5%
15	P239	-0.218Gf1	0.0%	1.5%	0.6%	-0.1%
16	P239	-0.218Gf2	0.4%	1.3%	3.4%	2.2%
17	P239	-0.037Gn	0.0%	-0.3%	-0.5%	-0.2%
18	P239	-0.037Gg	0.4%	0.6%	2.1%	1.3%
19	P239	-0.037Gf1	0.2%	1.9%	0.6%	-1.4%
20	P239	-0.037Gf2	0.0%	0.0%	0.0%	0.0%
21	P239	0.294Gn	-0.2%	0.8%	1.0%	0.7%
22	P239	0.294Gg	-0.3%	-2.2%	-0.2%	0.1%
23	P239	0.294Gf1	-0.2%	-3.2%	-0.7%	0.0%
24	P239	0.294Gf2	0.0%	0.0%	0.0%	0.0%

- Nubar changes appear reasonable
- Pu239 resonance parameters?

P239	nubar	1	0.0%	-0.1%	-0.2%	0.1%
P239	nubar	2	0.1%	-0.2%	-0.1%	0.3%
P239	nubar	3	0.1%	-0.1%	0.1%	0.3%
P239	nubar	4	0.1%	0.1%	0.6%	0.2%
P239	nubar	5	0.0%	0.1%	0.5%	0.1%
P239	nubar	6	0.0%	0.1%	0.3%	0.0%
P239	nubar	7	0.0%	0.1%	-0.2%	-0.1%
P239	nubar	8	0.0%	-0.1%	-0.5%	-0.1%
P239	nubar	9	0.0%	0.0%	-0.6%	-0.1%
P239	nubar	10	0.0%	0.0%	-0.2%	0.0%
P239	nubar	11	0.0%	0.0%	0.0%	0.0%
P239	nubar	12	0.0%	0.0%	0.0%	0.0%
P239	nubar	13	0.0%	0.0%	0.0%	0.0%
P239	nubar	14	0.0%	0.0%	-0.2%	-0.1%

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