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Reactivity loss and thermal standards: can JEFF-4T1 and ENDF/BVIII.0 be improved ?

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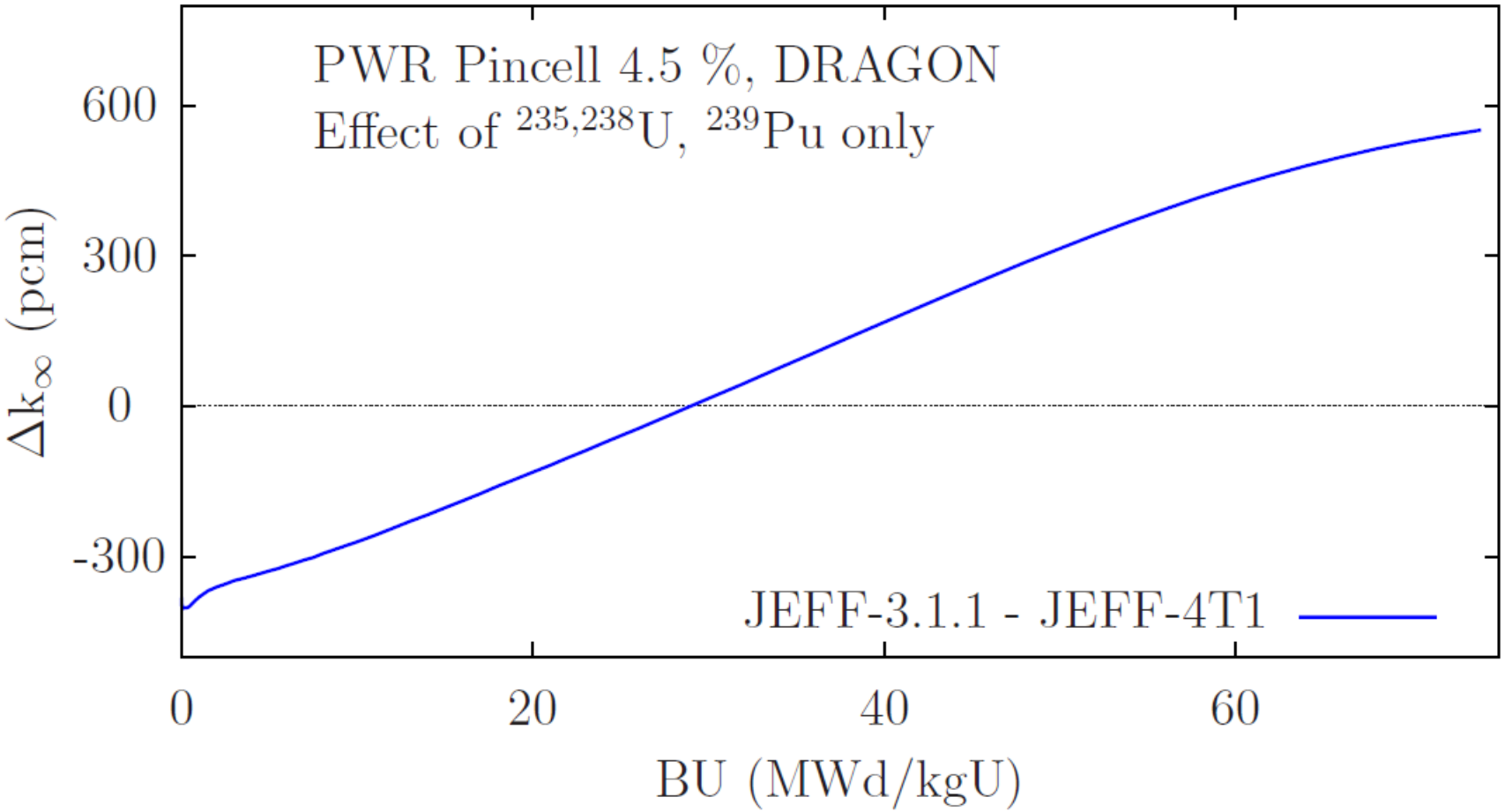
Summary

- Observations and questions for JEFF-4T1
- Conclusion for JEFF-4T1

- Observations and questions for ENDF/B-VIII.0
- Conclusion for ENDF/B-VIII.0

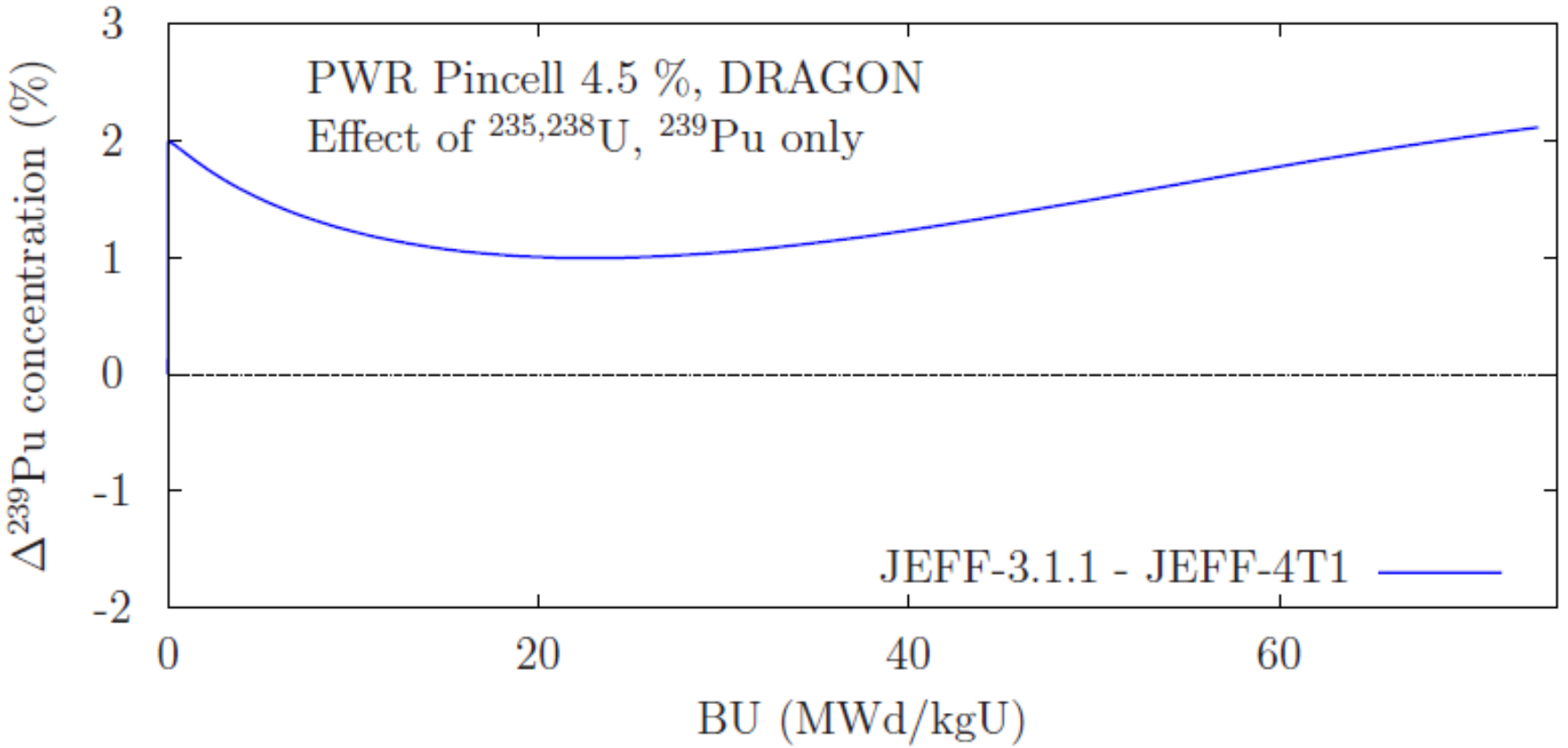
Main observation 1: JEFF-3.1.1 vs JEFF-4T1

- k_∞ reactivity loss



Main observation 2: JEFF-3.1.1 vs JEFF-4T1

- ^{239}Pu production loss



Main observation 3: JEFF-3.1.1 vs JEFF-4T1

- Mismatch between JEFF-4T1 and the standards

Cross section	Standard barns	JEFF311	JEFF4T1 prior barns
$^{235}U(n_{th},f)$	587.288 ± 1.351	585.062 (-2.226)	588.005 (+0.7)
$^{235}U(n_{th},\gamma)$	99.5 ± 1.3	98.7 (-0.8)	99.5 (+0.0)
$^{238}U(n_{th},\gamma)$	2.678 ± 0.016	2.695 (+0.017)	2.692 (+0.014)
$^{239}Pu(n_{th},f)$	752.371 ± 2.182	750.145 (-2.226)	749.771 (-2.6)
$^{239}Pu(n_{th},\gamma)$	269.8 ± 2.7	273.9 (+4.1)	271.0 (+1.2)
χ^2 (with k_{eff} & ^{239}Pu conc.)		1.5	2.1

Goal/question

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- Can we modify the RRR of JEFF-4T1 ^{235,238}U and ^{239}Pu to reproduce JEFF-3.1.1 k_∞, ^{239}Pu concentration and the thermal standards ?

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- JEFF-3.1.1 is believed to be the reference from industrial partners (reactivity and ^{239}Pu production)
- JEFF-3.3 and JEFF-4T1 are not performing as JEFF-3.1.1

- Can we modify the RRR of JEFF-4T1 ^{235,238}U and ^{239}Pu to reproduce JEFF-3.1.1 k_∞, ^{239}Pu concentration and the thermal standards ?

- Our sensitivity to k_∞ has identified 17 RRR parameters

	Isotope	Energy eV	Parameter	Prior eV (± 1 %)
1	^{239}Pu	-6.9087	Γ_{f1}	-0.9235
2	^{239}Pu	-0.219	Γ_n	$3.497e^{-5}$
3	^{239}Pu	+0.2956	Γ_γ	$39.82e^{-3}$
4	^{239}Pu	+0.2956	Γ_{f1}	$5.619e^{-2}$
5	^{235}U	-5.253	Γ_n	$1.217e^{-2}$
6	^{235}U	-5.253	Γ_γ	$3.679e^{-2}$
7	^{235}U	-5.253	Γ_{f1}	$1.956e^{-1}$
8	^{235}U	-5.253	Γ_{f2}	$-1.600e^{-1}$
9	^{235}U	-0.4808	Γ_γ	$3.922e^{-2}$
10	^{235}U	-0.432	Γ_n	$3.240e^{-5}$
11	^{235}U	-0.432	Γ_{f1}	$1.739e^{-1}$
12	^{238}U	+6.6742	Γ_n	$1.492e^{-3}$
13	^{238}U	+6.6742	Γ_γ	$2.271e^{-2}$
14	^{238}U	+20.871	Γ_n	$1.0076e^{-2}$
15	^{238}U	+20.871	Γ_γ	$2.275e^{-2}$
16	^{238}U	+36.682	Γ_n	$3.359e^{-2}$
17	^{238}U	+36.682	Γ_γ	$2.226e^{-2}$

Goal/question

- 2 methods applied, independently
  - TMC (random variations of the 17 parameters, ± 1%)
  - MOCABA (equivalent to GLLS, 17 parameters, ± 1%)

- Chi2 on k_∞, ^{239}Pu concentration and 5 standards

  (± 100 pcm, ± 1 %, and standard uncertainties)

	Isotope	Energy eV	Parameter	Prior eV (± 1 %)
1	^{239}Pu	-6.9087	Γ_{f1}	-0.9235
2	^{239}Pu	-0.219	Γ_n	$3.497e^{-5}$
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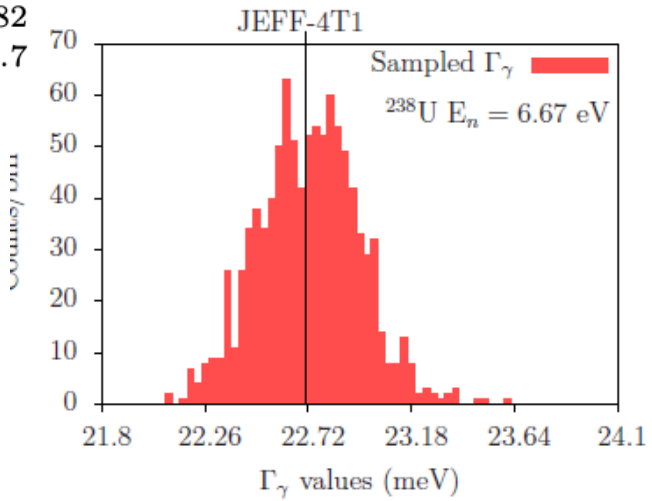
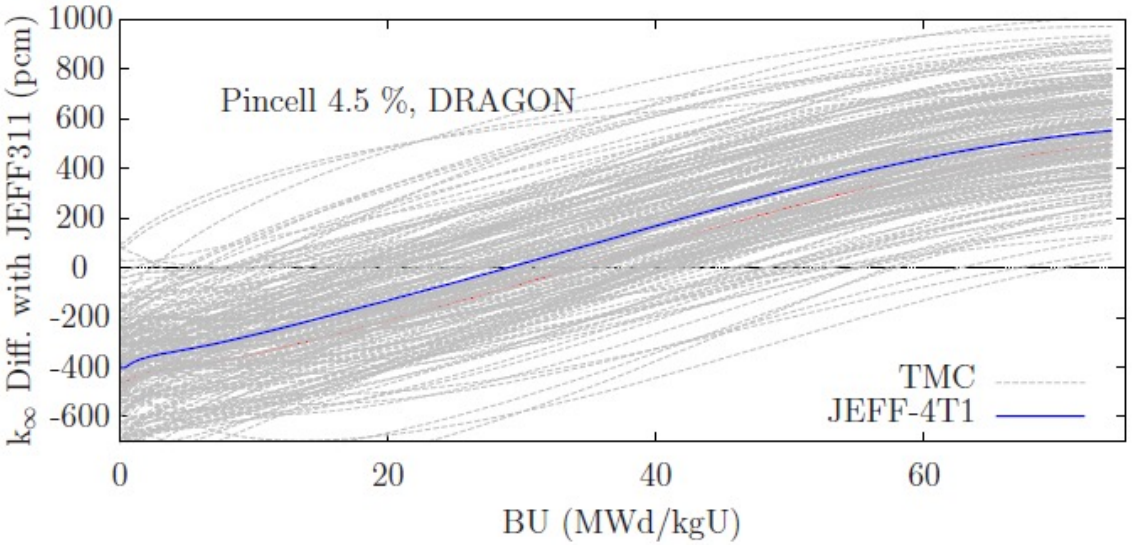
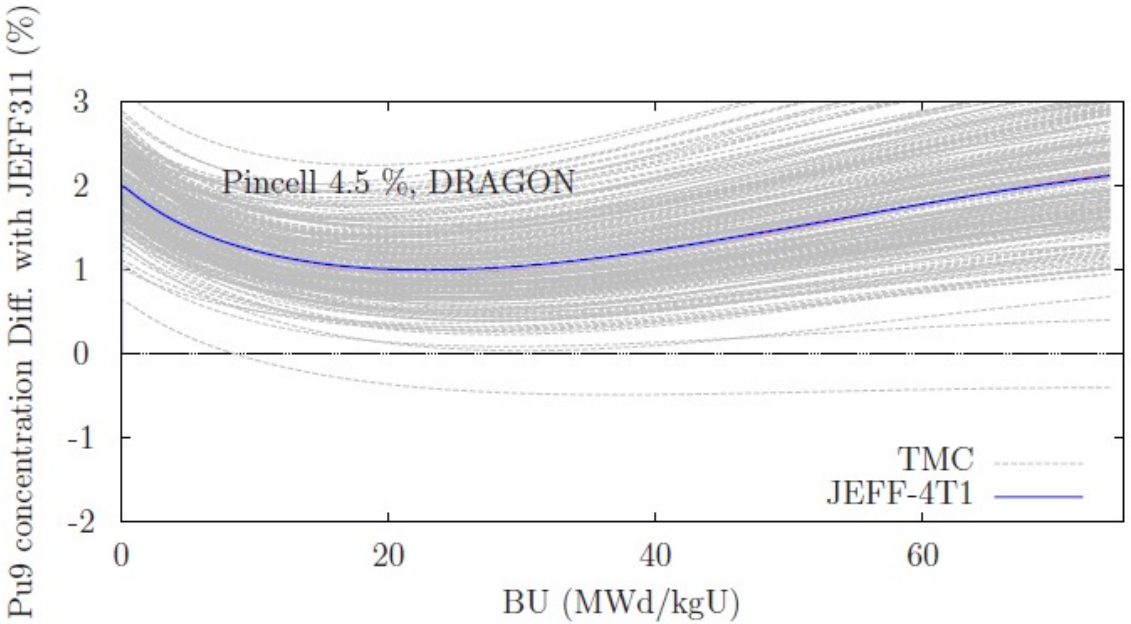
Cross section	Standard		
	barns		
^{235}U(n_{th},f)	587.288	±	1.351
^{235}U(n_{th},γ)	99.5	±	1.3
^{238}U(n_{th},γ)	2.678	±	0.016
^{239}Pu(n_{th},f)	752.371	±	2.182
^{239}Pu(n_{th},γ)	269.8	±	2.7

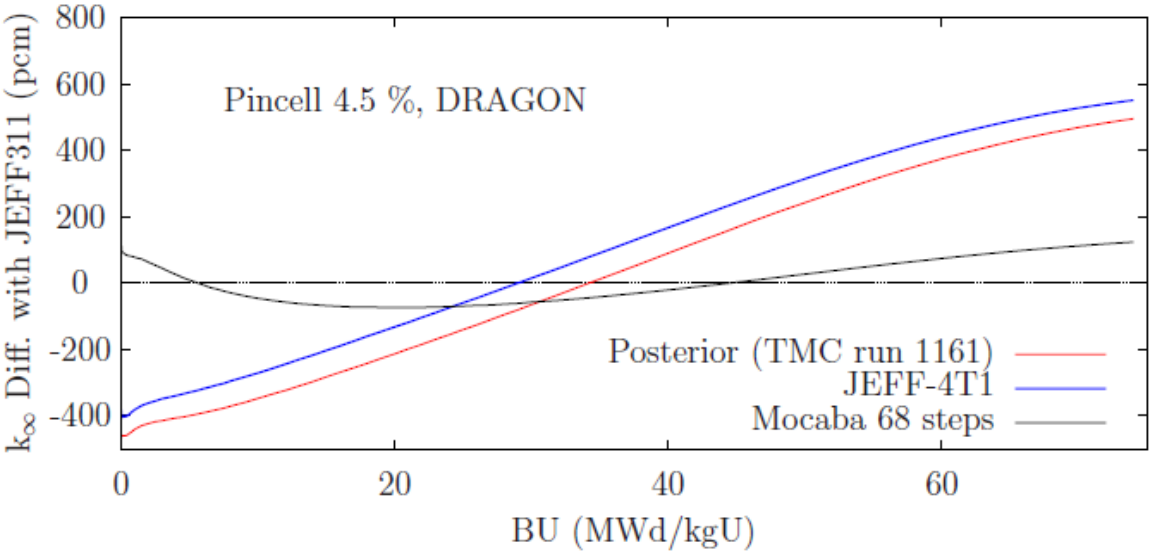


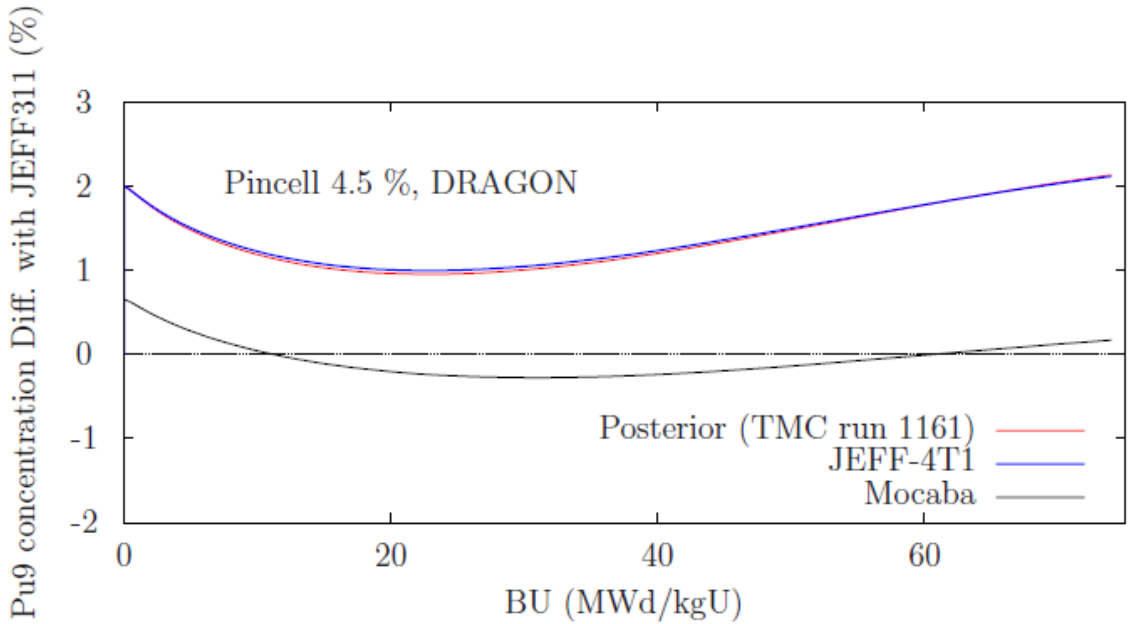
Sampling JEFF-4.T1 RRR 17 parameters





Best 17 parameters





Best 17 parameters

Cross section	Standard			JEFF311		JEFF4T1 prior		JEFF4T1 posterior TMC run 1161		JEFF4T1 posterior (Mocaba) 68 BU steps	
	barns					barns		barns		barns	
$^{235}U(n_{th},f)$	587.288	±	1.351	585.062	(-2.226)	588.005	(+0.7)	586.824	(-0.4)	584.260	(-3.0)
$^{235}U(n_{th},\gamma)$	99.5	±	1.3	98.7	(-0.8)	99.5	(+0.0)	100.4	(+0.9)	98.7	(-0.8)
$^{238}U(n_{th},\gamma)$	2.678	±	0.016	2.695	(+0.017)	2.692	(+0.014)	2.691	(+0.013)	2.752	(+0.074)
$^{239}Pu(n_{th},f)$	752.371	±	2.182	750.145	(-2.226)	749.771	(-2.6)	752.688	(+0.32)	753.357	(+0.99)
$^{239}Pu(n_{th},\gamma)$	269.8	±	2.7	273.9	(+4.1)	271.0	(+1.2)	270.2	(+0.4)	269.2	(-0.6)
χ^2 (with k_{eff} & ^{239}Pu conc.)				1.5		2.1		1.2		0.4 *(3.2)*	

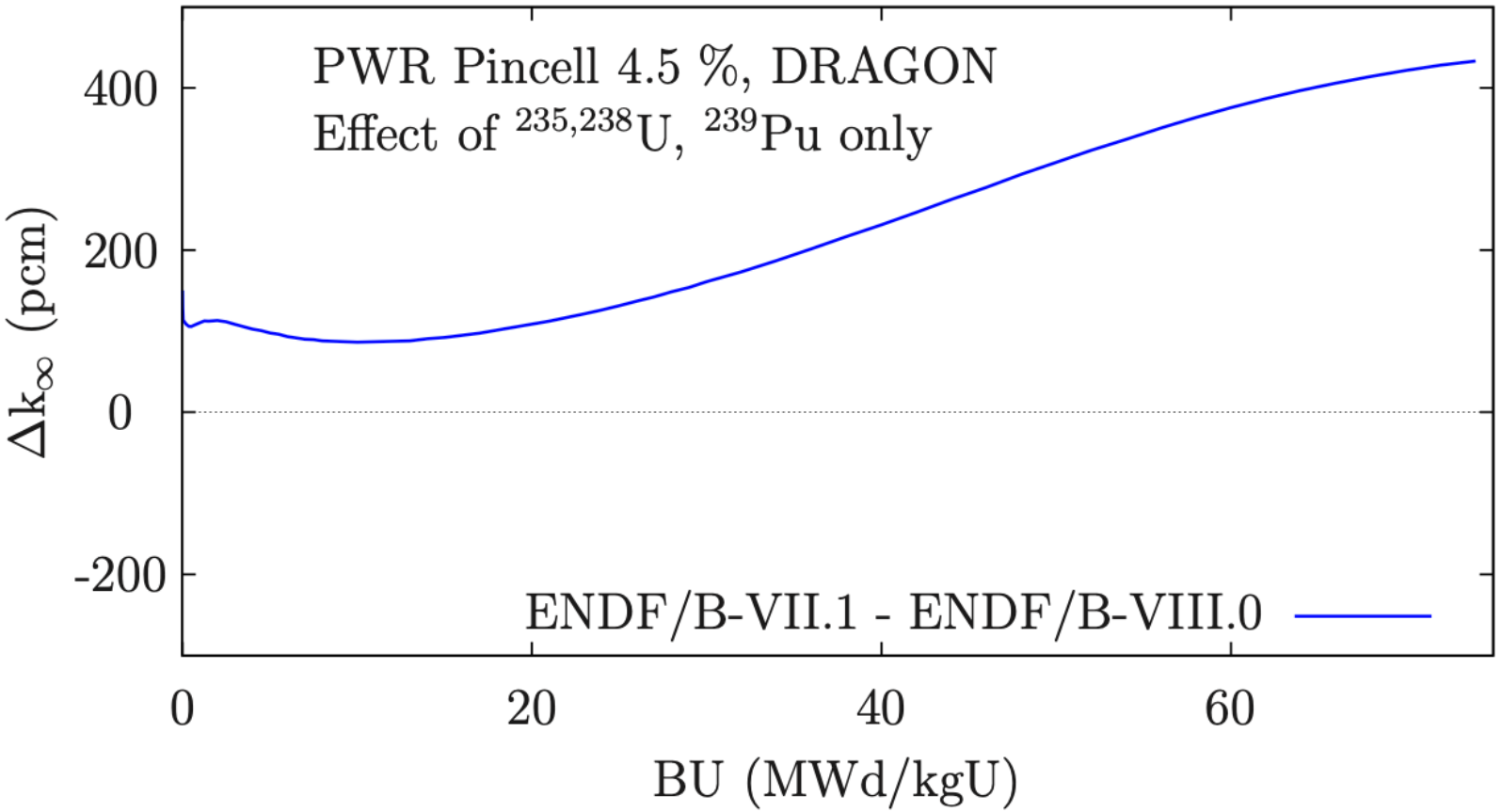
- TMC: modified JEFF4-T1 in good agreement with the standards, but not with k_∞ and ^{239}Pu
- Mocaba: contrary

- Conclusion: with the current JEFF-4T1 RRR for ^{235,238}U and ^{239}Pu, no agreement foreseen between k_∞, ^{239}Pu concentration, and the standard cross sections, while moderately changing the RRR parameters.

In the following slides, study with ENDF/B-VII.1 and ENDF/B-VIII.0

Main observation 1: ENDF/B-VII.1 vs ENDF/B-VIII.0

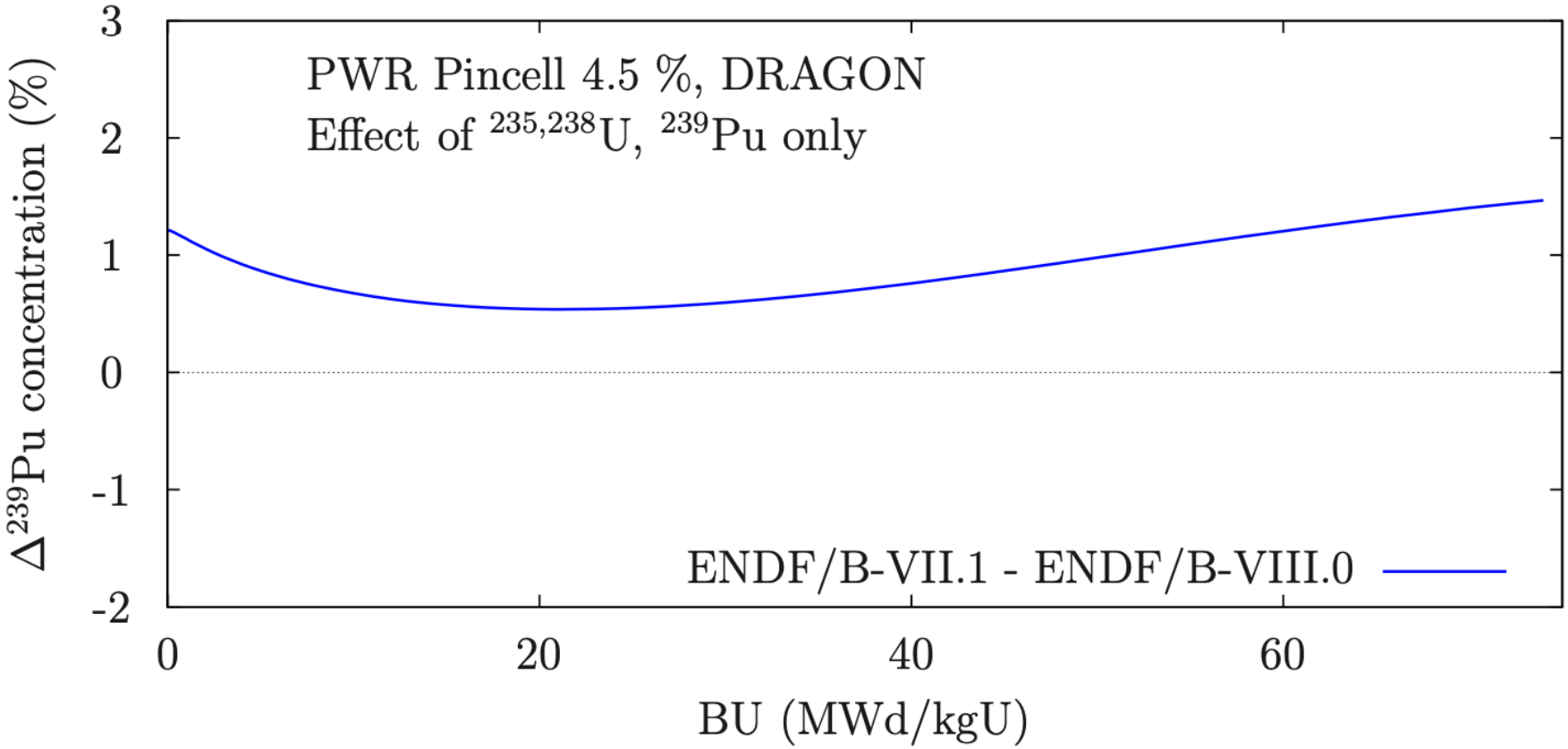
- k_∞ reactivity loss



- Note 1: RRR for ^{238}U and ^{239}Pu are the same in ENDF/B-VIII.0 and JEFF-4.T1
- Note 2: for ENDF/B-VIII.0, 21 RRR parameters are considered

Main observation 2: ENDF/B-VII.1 vs ENDF/B-VIII.0

- ^{239}Pu production loss



Main observation 3: ENDF/B-VII.1 vs ENDF/B-VIII.0

- Mismatch between ENDF/B-VIII.0 and the standards

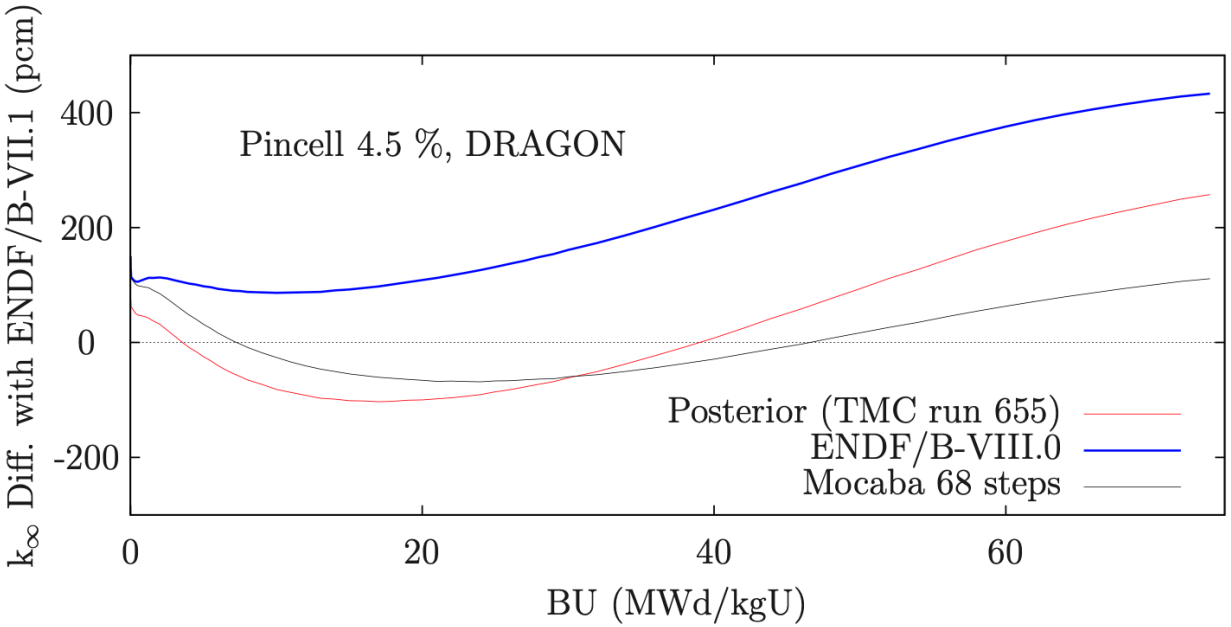
Cross section	Standard barns	ENDF/B-VII.1	ENDF/B-VIII.0 prior barns
$^{235}U(n_{th},f)$	587.288 ± 1.351	585.062 (-2.226)	586.884 (-0.4)
$^{235}U(n_{th},\gamma)$	99.5 ± 1.3	98.7 (-0.8)	99.4 (-0.1)
$^{238}U(n_{th},\gamma)$	2.678 ± 0.016	2.694 (+0.016)	2.692 (+0.014)
$^{239}Pu(n_{th},f)$	752.371 ± 2.182	751.309 (-1.062)	749.771 (-2.6)
$^{239}Pu(n_{th},\gamma)$	269.8 ± 2.7	271.8 (+2.0)	271.0 (+1.2)
χ^2 (with k_{eff} & ^{239}Pu conc.)		1.0	5.4

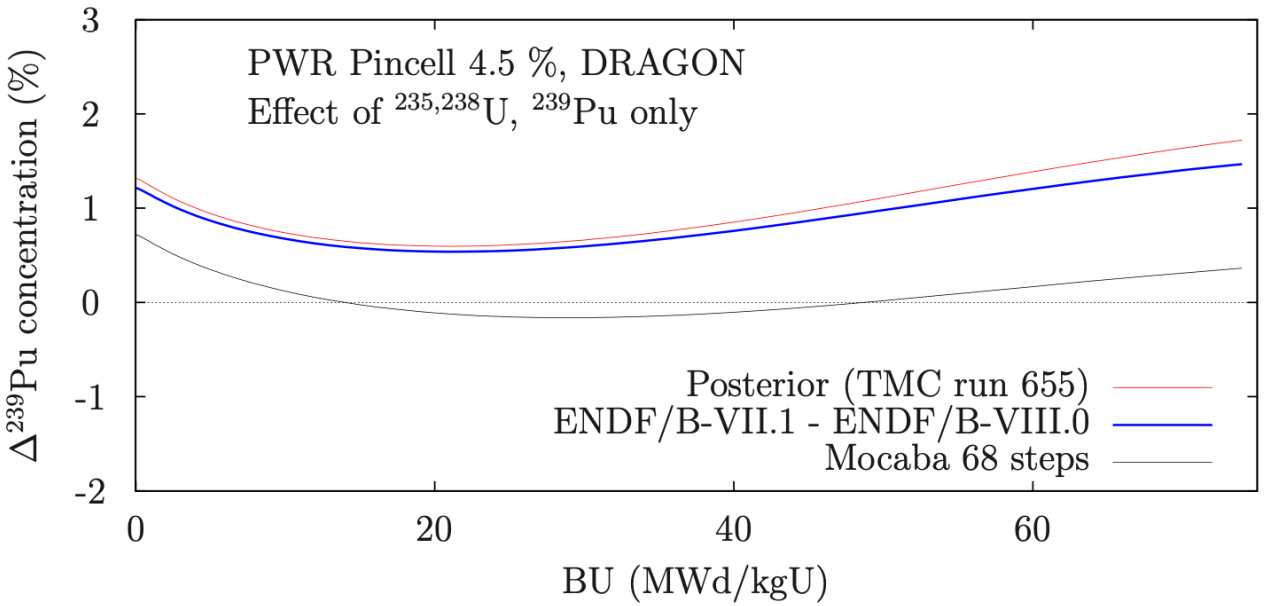
ENDF/B-VII.1 vs ENDF/B-VIII.0

- Same approach as for JEFF-3.1.1 and JEFF-4T1:
  - Randomly vary 21 most sensitive RRR parameters
  - Search agreement with the standards and with k_∞ and ^{239}Pu production (from ENDF/B-VII.1)

- Can a solution be found without changing too much the RRR of $^{235,238}U$ and ^{239}Pu ?

Best 21 parameters





Best 21 parameters

Cross section	Standard barns	ENDF/B-VII.1	ENDF/B-VIII.0 prior barns	ENDF/B-VIII.0 posterior TMC run 655 barns	ENDF/B-VIII.0 posterior (Mocaba) 68 BU steps barns
$^{235}U(n_{th},f)$	587.288 ± 1.351	585.062 (-2.226)	586.884 (-0.4)	587.905 (+0.6)	588.369 (+1.1)
$^{235}U(n_{th},\gamma)$	99.5 ± 1.3	98.7 (-0.8)	99.4 (-0.1)	99.4 (-0.1)	98.2 (-1.3)
$^{238}U(n_{th},\gamma)$	2.678 ± 0.016	2.694 (+0.016)	2.692 (+0.014)	2.690 (+0.012)	2.723 (+0.045)
$^{239}Pu(n_{th},f)$	752.371 ± 2.182	751.309 (-1.062)	749.771 (-2.6)	753.000 (+0.63)	752.747 (+0.4)
$^{239}Pu(n_{th},\gamma)$	269.8 ± 2.7	271.8 (+2.0)	271.0 (+1.2)	269.6 (-0.2)	268.9 (-0.9)
χ^2 (with k_{eff} & ^{239}Pu conc.)		1.0	5.4	0.5	1.0 *(4.1)*

- TMC: modified ENDF/B-VIII.0 in good agreement with the standards, but not with k_{eff}, Pu9
- Mocaba: contrary

- Conclusion:
  - with the current ENDF/B-VIII.0 RRR for ^{235,238}U and ^{239}Pu, no agreement foreseen between k_{eff}, Pu9 concentration, and the standard cross sections.
  - But the agreement is a bit better then for JEFF4-T1 (because the prior is a bit better)

Conclusion

- Both libraries (JEFF4-T1 and ENDF/B-VIII.0) provides different performances compared to their industry references (JEFF-3.1.1 and ENDF/B-VII.1)
  - Loss of reactivity
  - Loss of ^{239}Pu production

- The causes are partly from changes in the RRR of ^{235,238}U and ^{239}Pu.
- Both libraries share the same RRR for ^{238}U and ^{239}Pu.

- Changing moderately the RRR of ^{235,238}U and ^{239}Pu does not allow to correct for these deficiencies, and at the same time to agree with the 5 thermal standard cross sections.

Backup slides

Backup slides

Table 1: Parameters for the JEFF4T1 library (prior). Posterior values obtained based on k_{eff}, thermal values (standards), and ^{239}Pu production. 1000 random files are used. 7 partial chi2 for TMC, one single chi2 for Mocaba.

	Isotope	Energy eV	Parameter	Prior eV (± 1 %)	Posterior variations TMC (run 1161)		Posterior Uncertainty variations Mocaba 68 BU steps		
1	^{239}Pu	-6.9087	Γ_{f1}	-0.9235	-0.9244	+0.1 %	-0.9238	± 0.96 %	-0.01 %
2	^{239}Pu	-0.219	Γ_n	$3.497e^{-5}$	$3.464e^{-5}$	-0.9 %	$3.482e^{-5}$	± 0.75 %	-0.4 %
3	^{239}Pu	+0.2956	Γ_γ	$39.82e^{-3}$	$39.67e^{-3}$	-0.4 %	$39.48e^{-3}$	± 0.43 %	-0.9 %
4	^{239}Pu	+0.2956	Γ_{f1}	$5.619e^{-2}$	$5.711e^{-2}$	+1.6 %	$5.695e^{-2}$	± 0.64 %	+1.3 %
5	^{235}U	-5.253	Γ_n	$1.217e^{-2}$	$1.203e^{-2}$	-1.2 %	$1.206e^{-2}$	± 0.82 %	-0.9 %
6	^{235}U	-5.253	Γ_γ	$3.679e^{-2}$	$3.749e^{-2}$	+1.9 %	$3.656e^{-2}$	± 0.96 %	-0.6 %
7	^{235}U	-5.253	Γ_{f1}	$1.956e^{-1}$	$1.943e^{-1}$	-0.7 %	$1.955e^{-1}$	± 0.92 %	-0.05 %
8	^{235}U	-5.253	Γ_{f2}	$-1.600e^{-1}$	$-1.596e^{-1}$	+0.2 %	$-1.599e^{-1}$	± 0.97 %	+0.06 %
9	^{235}U	-0.4808	Γ_γ	$3.922e^{-2}$	$3.997e^{-2}$	+1.9 %	$3.887e^{-2}$	± 0.91 %	-0.9 %
10	^{235}U	-0.432	Γ_n	$3.240e^{-5}$	$3.259e^{-5}$	+0.6 %	$3.219e^{-5}$	± 0.86 %	-0.6 %
11	^{235}U	-0.432	Γ_{f1}	$1.739e^{-1}$	$1.758e^{-1}$	+1.1 %	$1.739e^{-1}$	± 0.90 %	+0.01 %
12	^{238}U	+6.6742	Γ_n	$1.492e^{-3}$	$1.504e^{-3}$	+0.8 %	$1.518e^{-3}$	± 0.82 %	+1.7 %
13	^{238}U	+6.6742	Γ_γ	$2.271e^{-2}$	$2.248e^{-2}$	-1.0 %	$2.302e^{-2}$	± 0.83 %	+1.3 %
14	^{238}U	+20.871	Γ_n	$1.0076e^{-2}$	$1.0088e^{-2}$	+0.1 %	$1.0194e^{-2}$	± 0.97 %	+1.1 %
15	^{238}U	+20.871	Γ_γ	$2.275e^{-2}$	$2.231e^{-2}$	-2.0 %	$2.298e^{-2}$	± 0.96 %	+1.0 %
16	^{238}U	+36.682	Γ_n	$3.359e^{-2}$	$3.404e^{-2}$	+1.3 %	$3.404e^{-2}$	± 0.97 %	+1.3 %
17	^{238}U	+36.682	Γ_γ	$2.226e^{-2}$	$2.258e^{-2}$	+1.4 %	$2.267e^{-2}$	± 0.95 %	+1.8 %

Backup slides

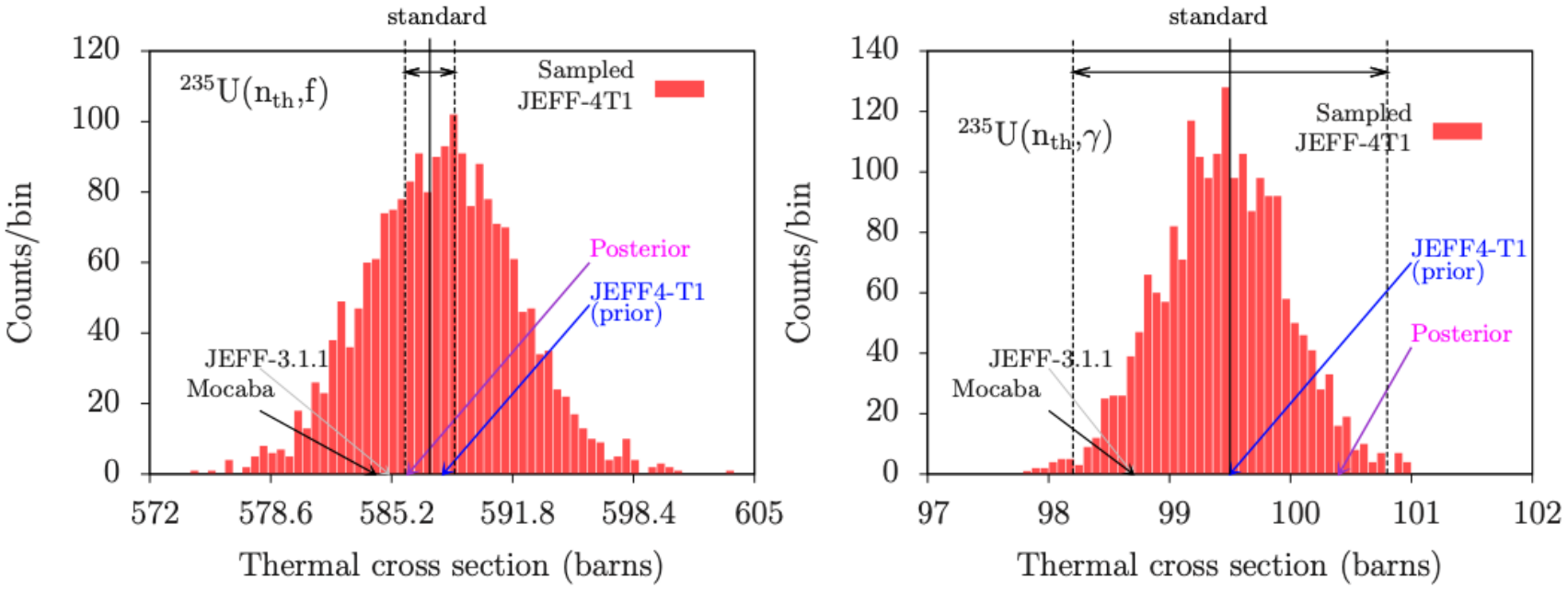


Figure 2: Prior (JEFF4-T1) and posterior thermal fission and capture cross sections for ^{235}U from the TMC approach.

Backup slides

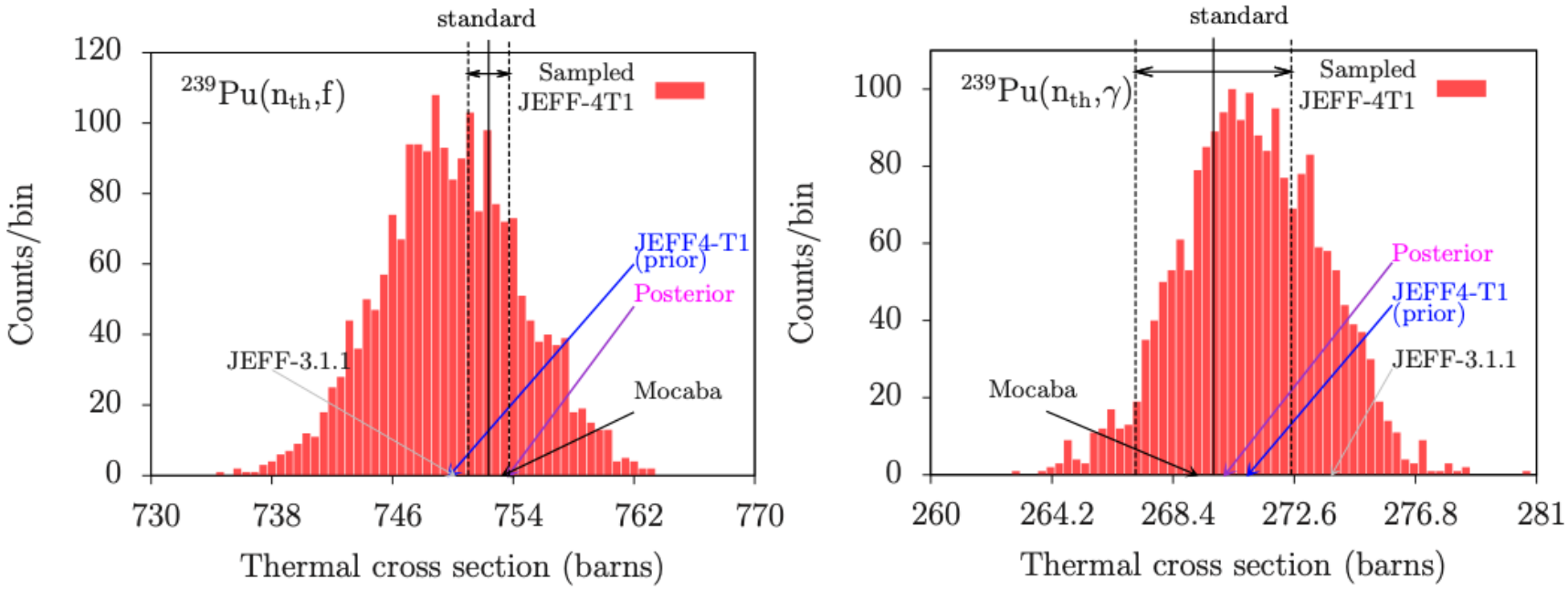


Figure 3: Prior (JEFF4-T1) and posterior thermal fission and capture cross sections for ^{239}Pu from the TMC approach.

Backup slides

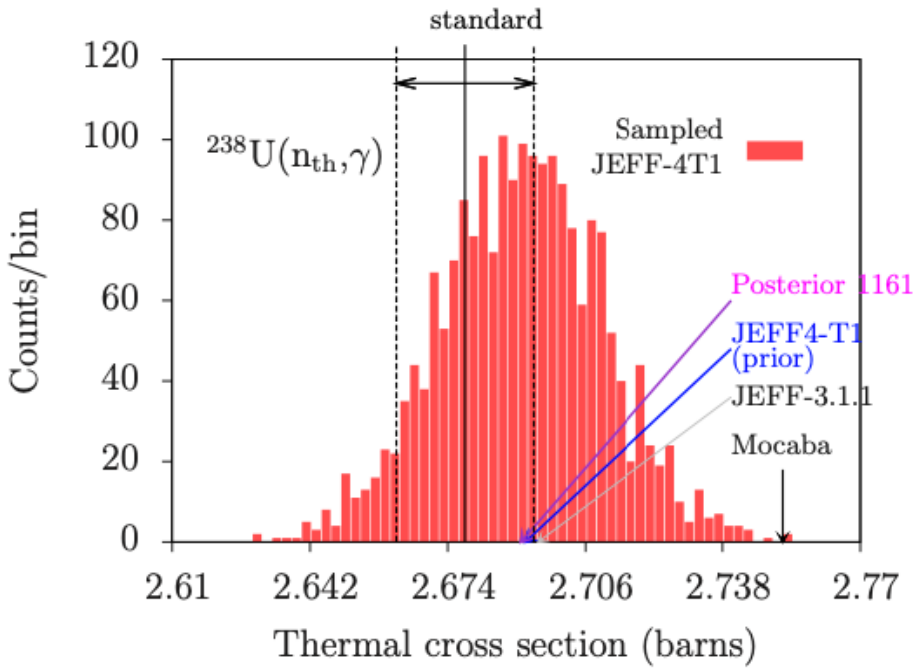


Figure 4: Prior (JEFF4-T1) and posterior thermal capture cross section for ^{238}U from the TMC approach.

Backup slides

Table 3: Parameters for the ENDF/B-VIII.0 library (prior). Posterior values obtained based on k_{eff}, thermal values (standards), and ^{239}Pu production. 1000 random files are used. 7 partial chi2 for TMC, one single chi2 for Mocaba. ^{239}Pu and ^{238}U contains the same resonances as in JEFF-4T1.

	Isotope	Energy eV	Parameter	Prior eV (± 1 %)	Posterior variations TMC (run 655)		Posterior Uncertainty variations Mocaba 68 BU steps		
1	^{239}Pu	-6.9087	Γ_{f1}	-0.9235	-0.9290	-0.6 %	-0.9151	± 0.97 %	+0.9 %
2	^{239}Pu	-0.219	Γ_n	$3.497e^{-5}$	$3.495e^{-5}$	-0.1 %	$3.484e^{-5}$	± 0.98 %	-0.4 %
3	^{239}Pu	+0.2956	Γ_n	$7.947e^{-5}$	$7.935e^{-5}$	-0.2 %	$7.976e^{-5}$	± 0.99 %	+0.4 %
4	^{239}Pu	+0.2956	Γ_γ	$39.82e^{-3}$	$39.61e^{-3}$	-0.5 %	$39.99e^{-3}$	± 0.97 %	+0.4 %
5	^{239}Pu	+0.2956	Γ_{f1}	$5.619e^{-2}$	$5.667e^{-2}$	+0.8 %	$5.548e^{-2}$	± 0.97 %	-1.3 %
6	^{235}U	-5.224	Γ_n	$1.146e^{-2}$	$1.154e^{-2}$	+0.7 %	$1.126e^{-2}$	± 0.75 %	-1.8 %
7	^{235}U	-5.224	Γ_γ	$5.548e^{-2}$	$5.465e^{-2}$	-1.5 %	$5.558e^{-2}$	± 0.93 %	+0.2 %
8	^{235}U	-5.224	Γ_{f1}	$2.049e^{-1}$	$2.043e^{-1}$	-0.3 %	$2.072e^{-1}$	± 0.87 %	+1.1 %
9	^{235}U	-0.4826	Γ_γ	$2.536e^{-2}$	$2.539e^{-2}$	+0.1 %	$2.502e^{-2}$	± 0.89 %	-1.3 %
10	^{235}U	-0.4826	Γ_{f2}	$-8.635e^{-2}$	$-8.612e^{-2}$	+0.3 %	$-8.685e^{-2}$	± 0.85 %	+0.6 %
11	^{235}U	-0.4291	Γ_n	$3.260e^{-5}$	$3.264e^{-5}$	+0.1 %	$3.272e^{-5}$	± 0.87 %	+0.4 %
12	^{235}U	-0.4291	Γ_γ	$3.513e^{-2}$	$3.529e^{-2}$	+0.4 %	$3.473e^{-2}$	± 0.93 %	-1.1 %
13	^{235}U	-0.4291	Γ_{f1}	$1.206e^{-1}$	$1.209e^{-1}$	+0.2 %	$1.195e^{-1}$	± 0.92 %	-0.9 %
14	^{235}U	+0.2684	Γ_n	$4.271e^{-6}$	$4.296e^{-6}$	+0.6 %	$4.189e^{-6}$	± 0.94 %	-1.9 %
15	^{235}U	+0.2684	Γ_γ	$4.732e^{-2}$	$4.761e^{-2}$	+0.6 %	$4.719e^{-2}$	± 0.90 %	-0.3 %
16	^{238}U	+6.6742	Γ_n	$1.492e^{-3}$	$1.483e^{-3}$	-0.6 %	$1.545e^{-3}$	± 0.74 %	+3.4 %
17	^{238}U	+6.6742	Γ_γ	$2.271e^{-2}$	$2.272e^{-2}$	+0.1 %	$2.300e^{-2}$	± 0.89 %	+1.3 %
18	^{238}U	+20.871	Γ_n	$1.0076e^{-2}$	$9.985e^{-3}$	-0.9 %	$1.0313e^{-2}$	± 0.93 %	+2.3 %
19	^{238}U	+20.871	Γ_γ	$2.275e^{-2}$	$2.319e^{-2}$	+1.9 %	$2.273e^{-2}$	± 0.96 %	-0.1 %
20	^{238}U	+36.682	Γ_n	$3.359e^{-2}$	$3.338e^{-2}$	-0.6 %	$3.404e^{-2}$	± 0.92 %	+1.3 %
21	^{238}U	+36.682	Γ_γ	$2.226e^{-2}$	$2.241e^{-2}$	+0.7 %	$2.301e^{-2}$	± 0.86 %	+3.2 %

Backup slides

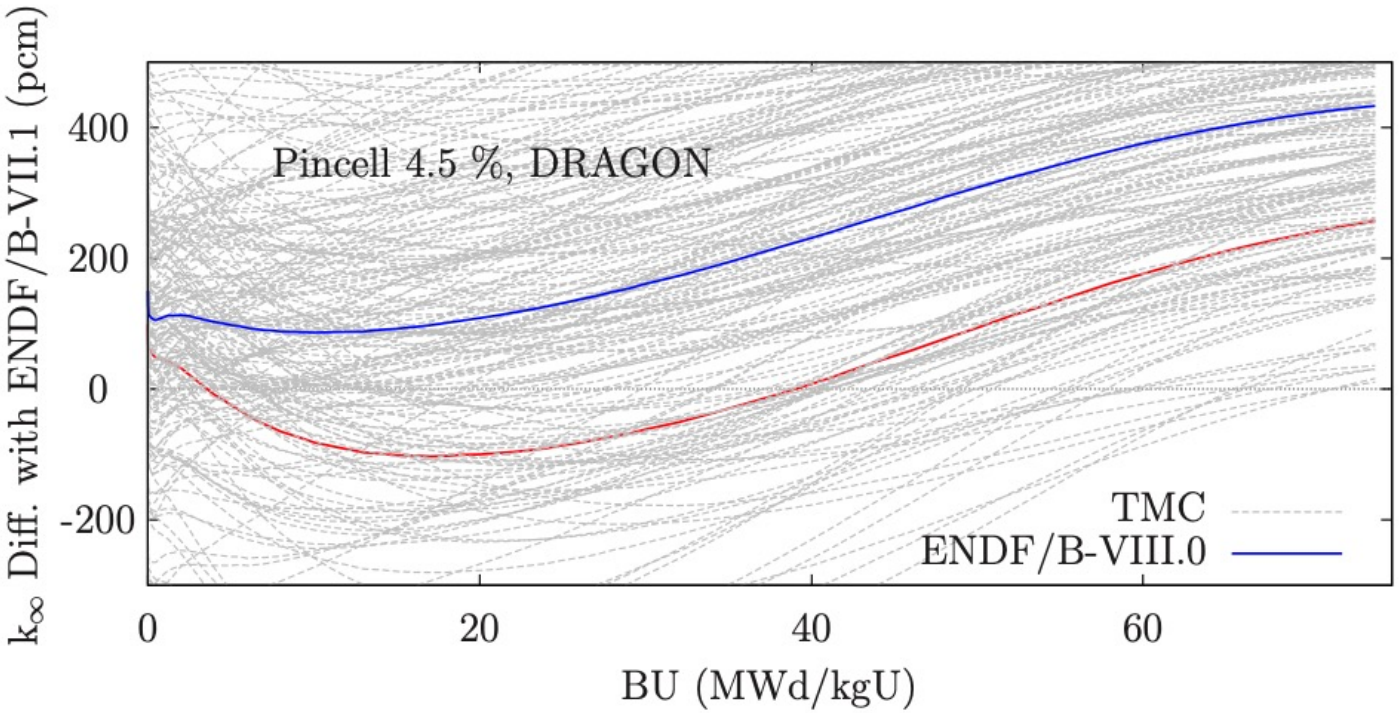


Figure 9: Difference for k_∞ with respect to ENDF/B-VII.1, for Pu9, U5 and U8 for the TMC random runs.

Backup slides

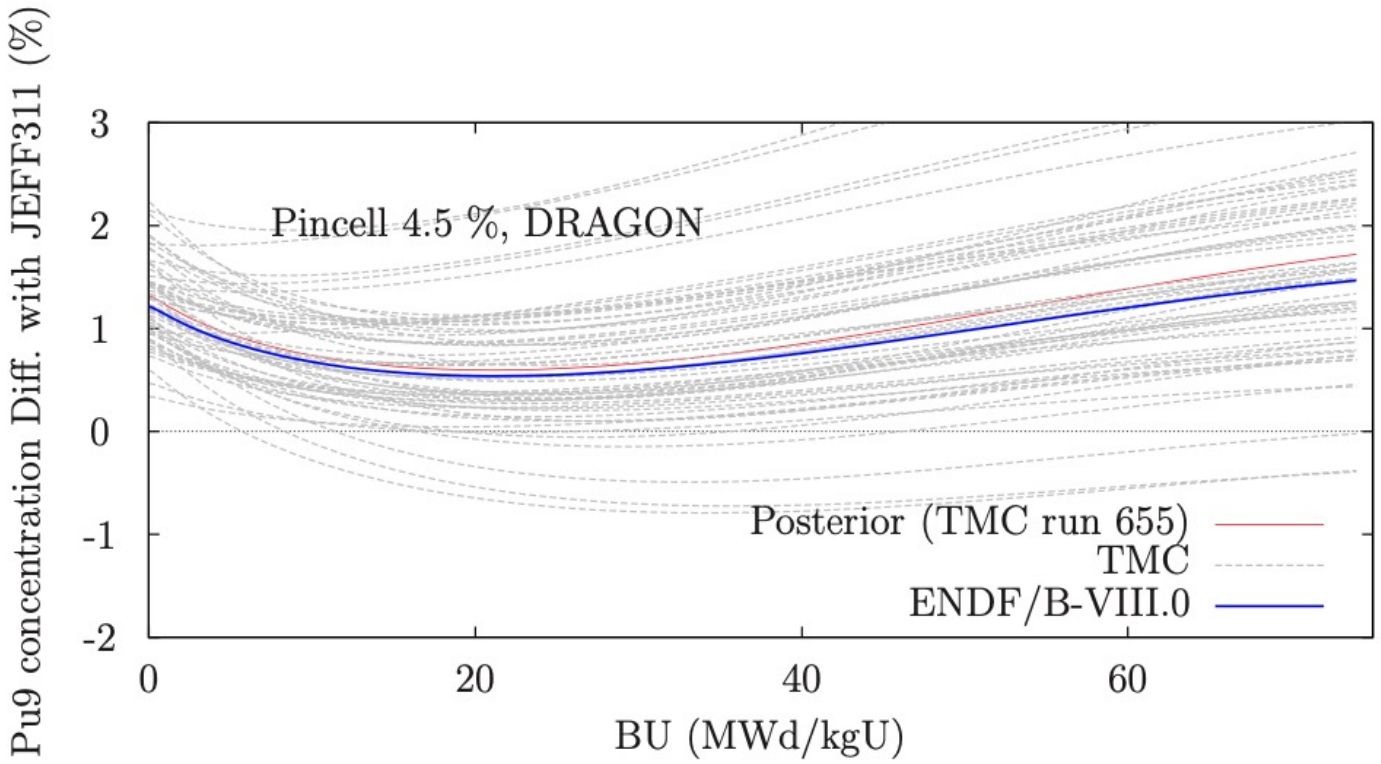


Figure 10: Difference for the Pu9 concentration with respect to ENDF/B-VII.1, for Pu9, U5 and U8.

Backup slides

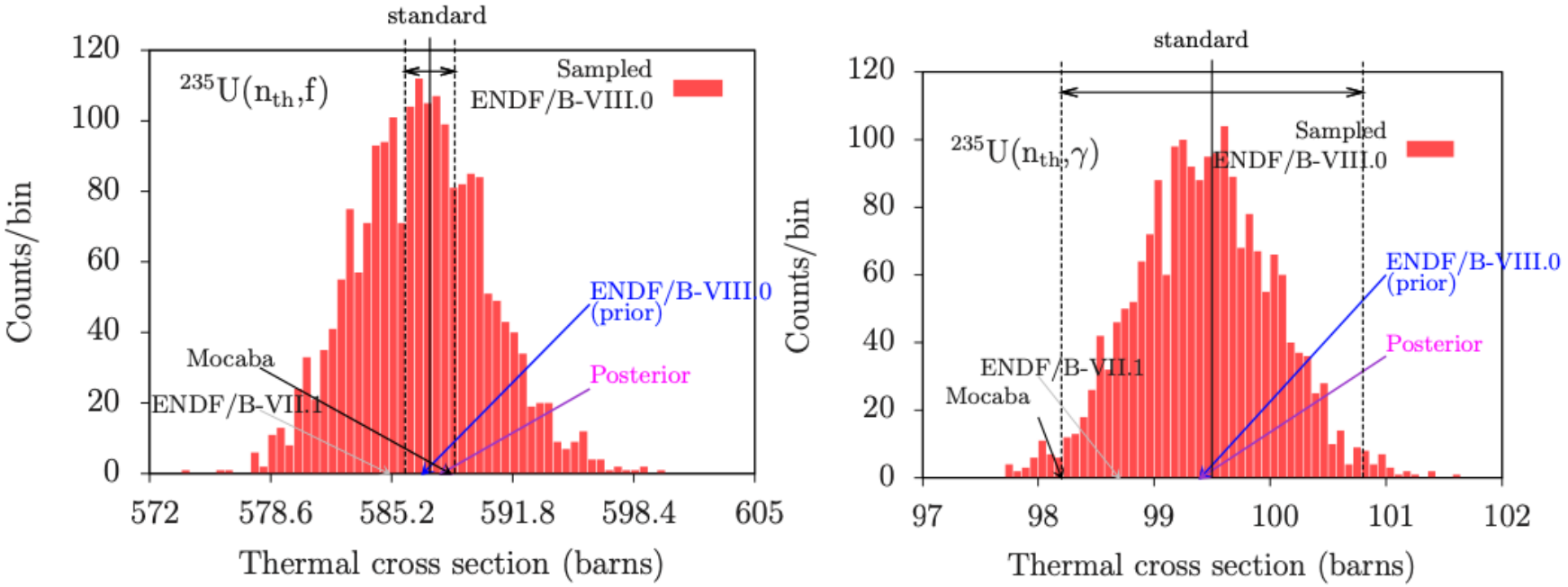


Figure 13: Prior (ENDF/B-VIII.0) and posterior thermal fission and capture cross sections for ^{235}U from the TMC approach.

Backup slides

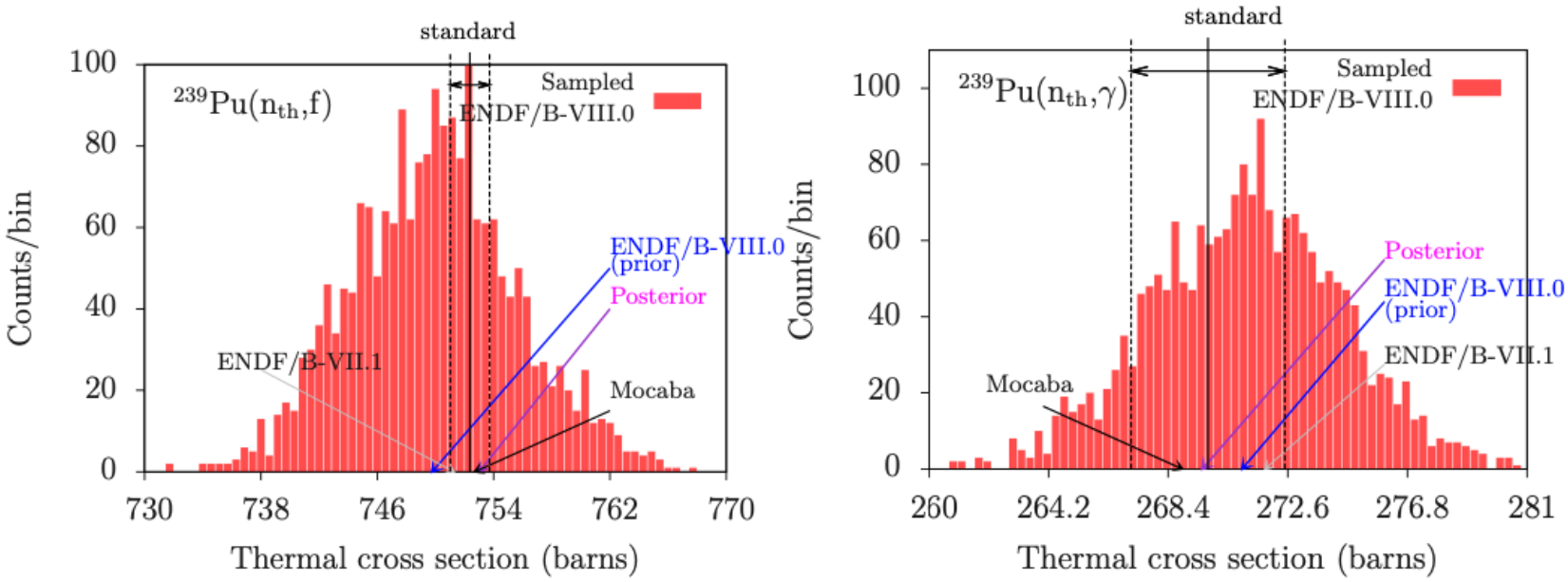


Figure 14: Prior (ENDF/B-VIII.0) and posterior thermal fission and capture cross sections for ^{239}Pu from the TMC approach.

Backup slides

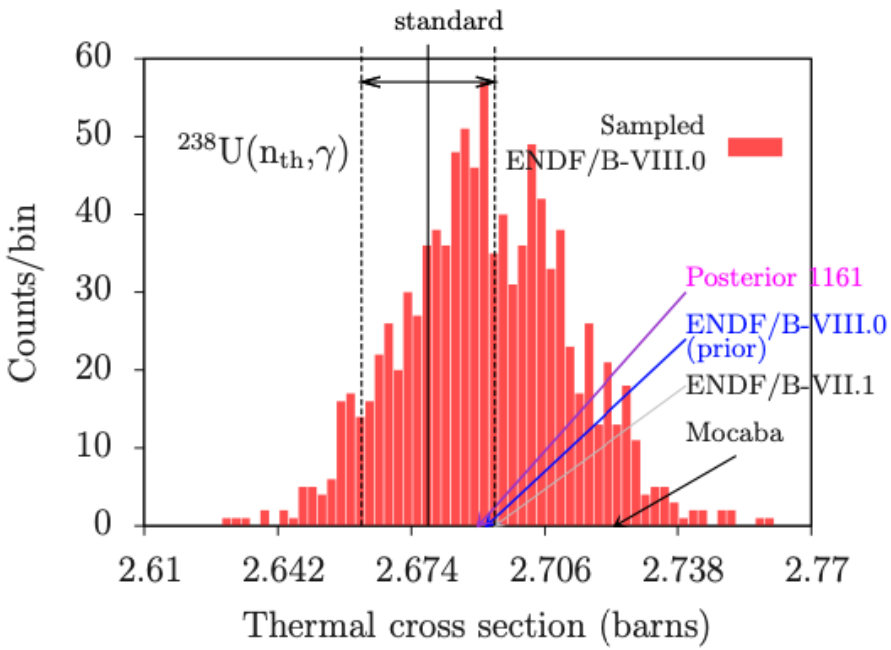
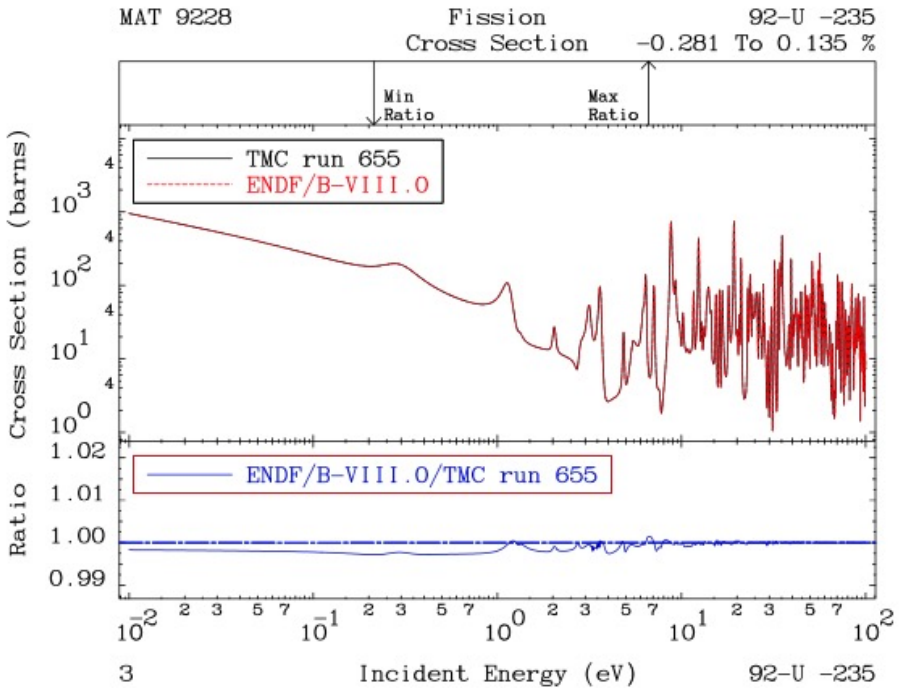
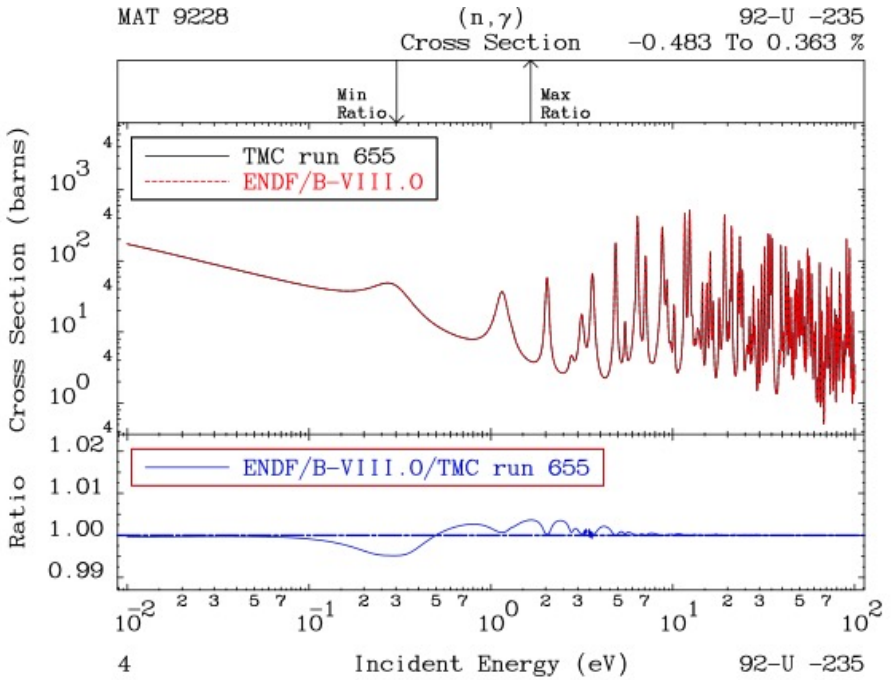


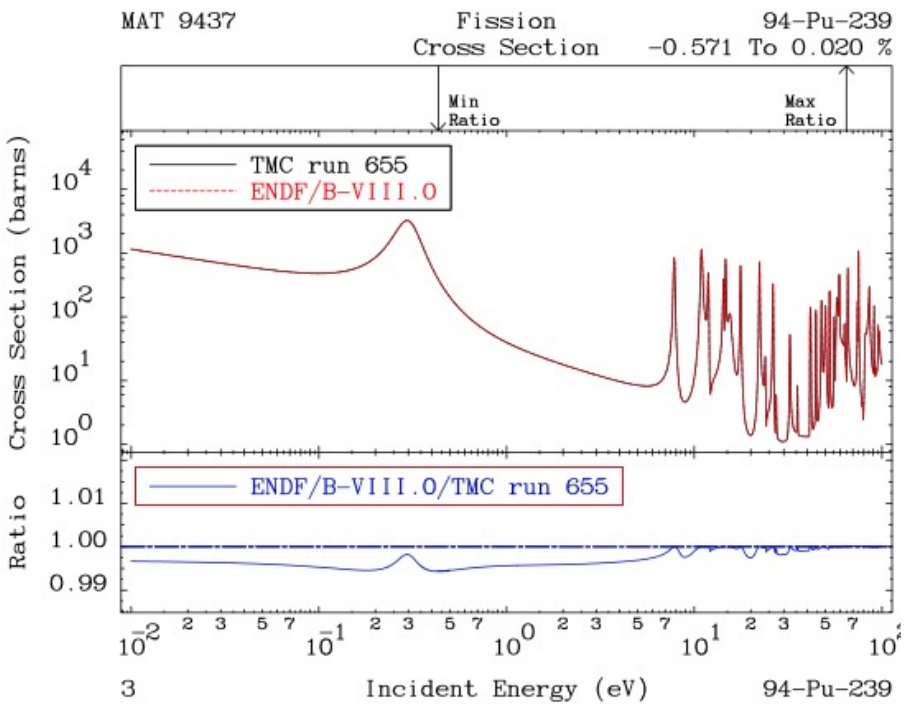
Figure 15: Prior (ENDF/B-VIII.0) and posterior thermal capture cross section for ^{238}U from the TMC approach.

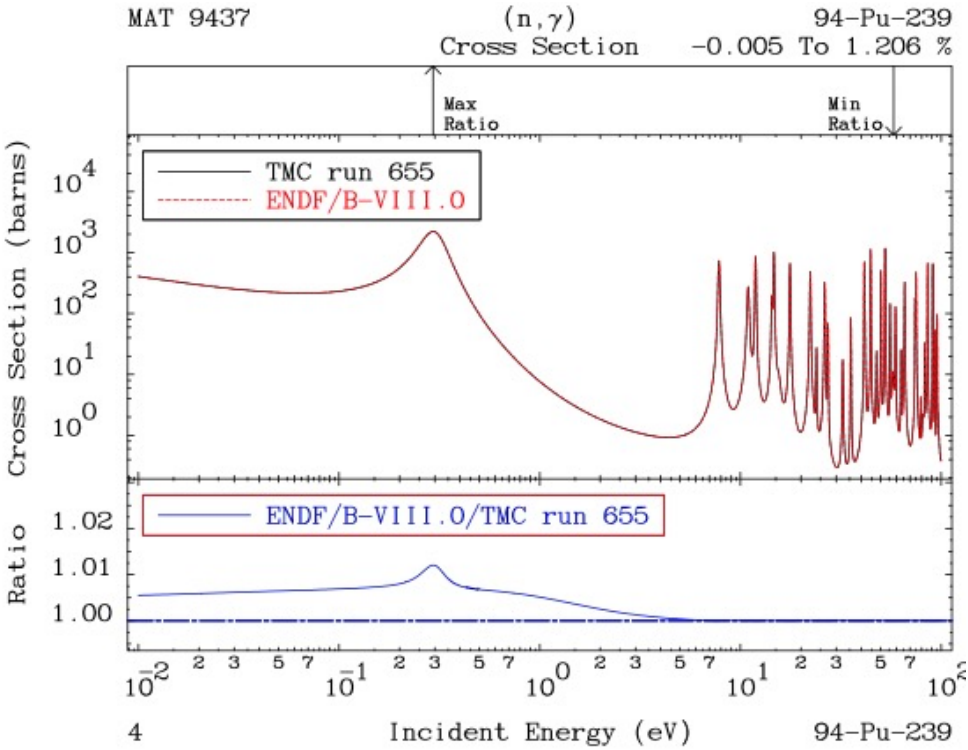
Backup slides





Backup slides





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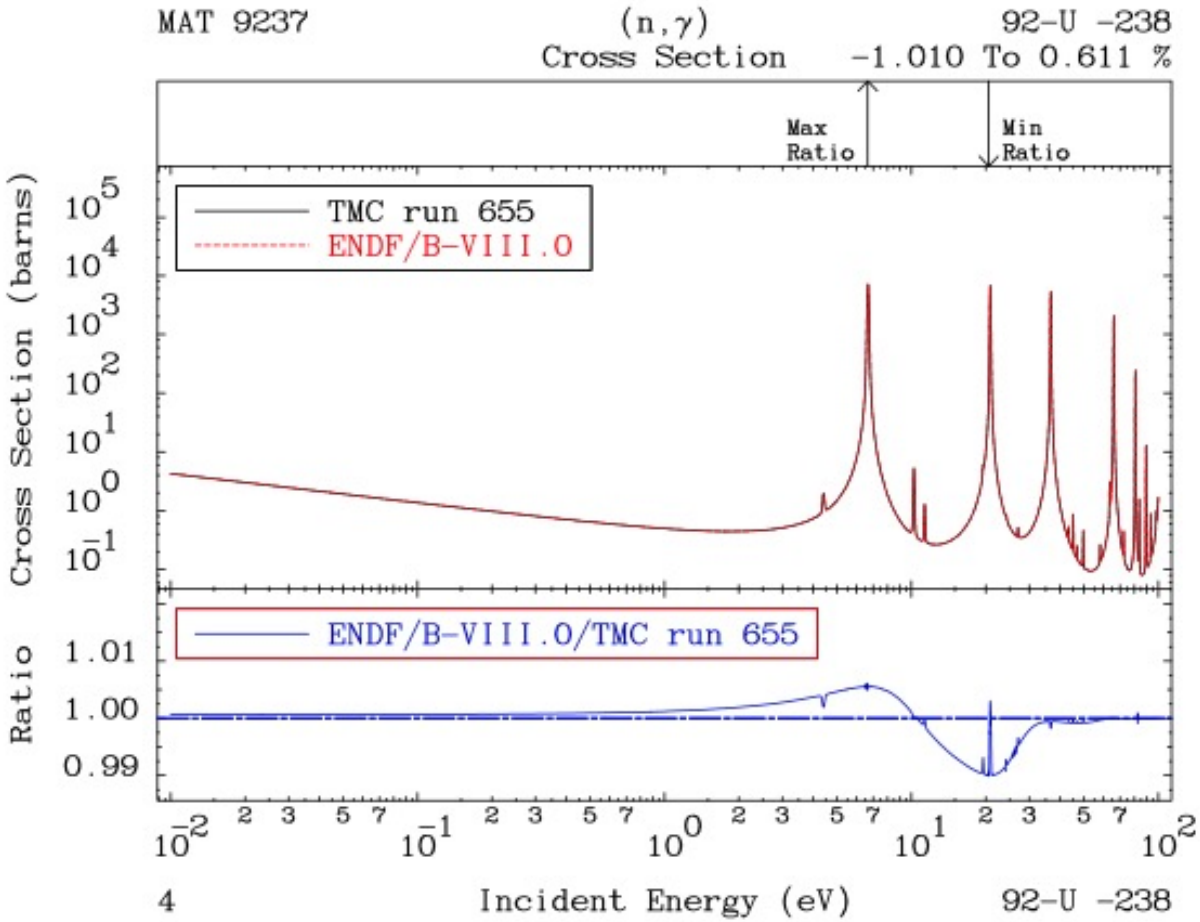

Figure 18: Comparison of ^{238}U(n,γ) between ENDF/B-VIII.0 and the file TMC-655.

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Wir schaffen Wissen – heute für morgen