

Benchmarking and Validation activities within JEFF Project

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OECD Nuclear Energy Agency
Data Bank

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Benchmarking and Validation Activities

- ❑ Paper in ND2016

Benchmarking and Validation Activities within JEFF Project

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❑ 14 JEFF Institutions !!!

Abstract. The challenge for any nuclear data evaluation project is to periodically release a revised, fully consistent and complete library, with all needed data and covariances, and ensure that it is robust and reliable for a variety of applications. Within an evaluation effort, benchmarking activities play an important role in validating proposed libraries. The Joint Evaluated Fission and Fusion (JEFF) Project aims to provide such a nuclear data library, and thus, requires a coherent and efficient benchmarking process. The aim of this paper is to present the activities carried out by the new JEFF Benchmarking and Validation Working Group, and to describe the role of the NEA Data Bank in this context. The paper will also review the status of preliminary benchmarking for the next JEFF-3.3 candidate cross-section files.

Main changes in JEFF-3.3 beta for criticality

Table 1 Main changes in JEFF3.3 beta files for criticality

	JEFF-3.3T2	JEFF-3.3T2P	JEFF-3.3T3
Pu239	JEFF-3.3T2	JEFF-3.3T2	JEFF-3.3T2
U235	JEFF-3.3T2	JEFF-3.3T2	JEFF-3.3T2
U238	JEFF-3.3T2	JEFF-3.3T2+RR/JRC	JEFF-3.3T2+RR-JRC
O16	ENDF/B-VII.1	O16-Luiz	O16-Luiz
TSLs	JEFF-3.1	H2O Bariloche D2OBariloche	H2O Bariloche D2OBariloche
Cu	ENDF/B-VII.1+RR/JRC	ENDF/B-VII.1+RR/JRC	KIT-revised + RR/Sobes&Luiz
Zr	TENDL-2015	JEFF-3.3T2=TENDL-2015	KIT
Fe54/56	JEFF-3.2	JEFF-3.2	ENDF/B-VIIIb4
W	JEFF-3.2	JEFF-3.2	JEFF-3.2
Be	JEFF-3.2	JEFF-3.2	JEFF-3.2
C	JEFF-3.2	JEFF-3.2	JEFF-3.2
Ni	JEFF-3.2	JEFF-3.2	JEFF-3.2
Al	JEFF-3.2	JEFF-3.2	JEFF-3.2
Th232	JEFF-3.2	JEFF-3.2	JEFF-3.2

1. Criticality Benchmarking with ICSBEP

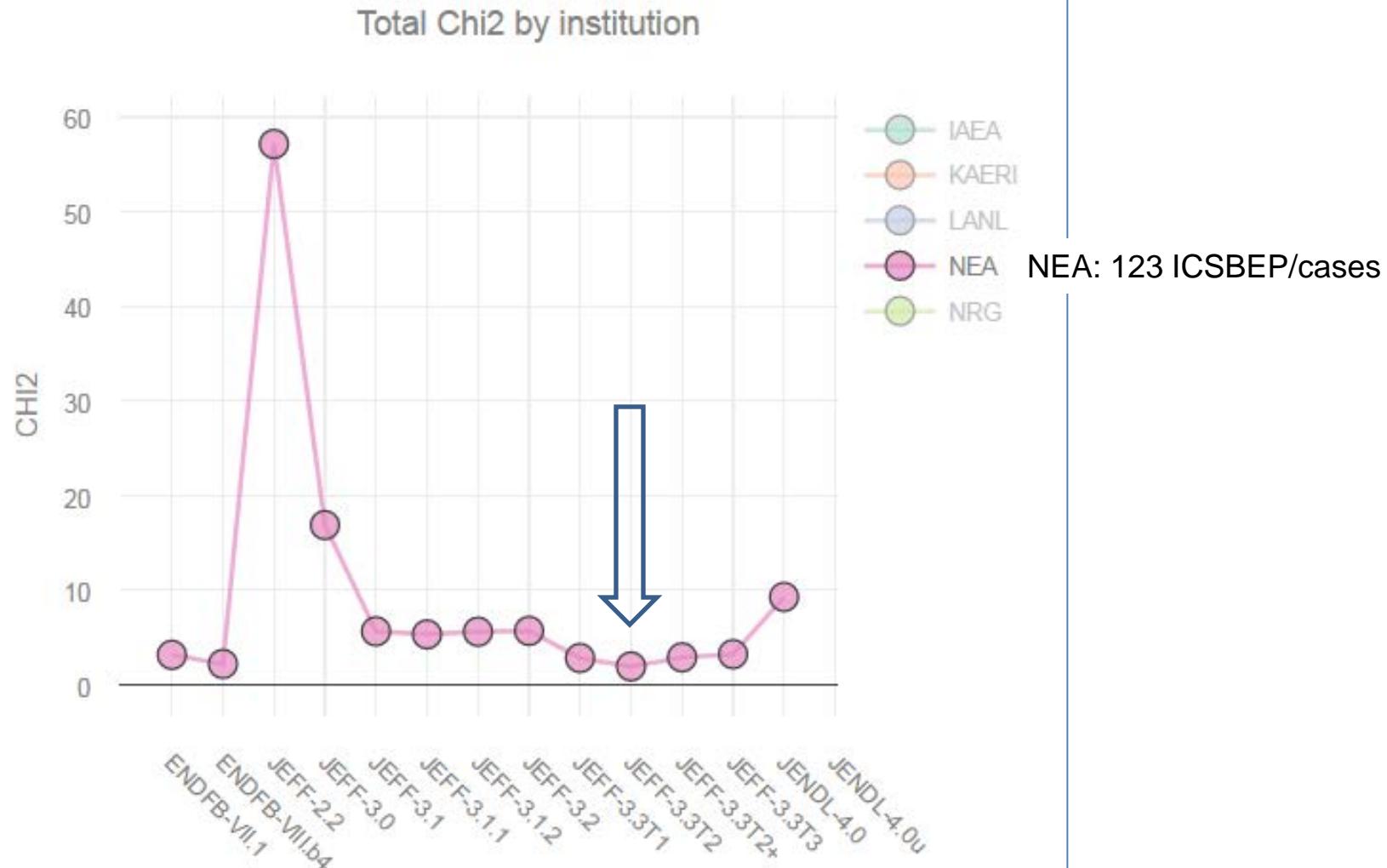
- ❑ NEA Validation Suite
 (R.D. Mosteller, 119 cases
 + 4 additional Benchmarks)

- ❑ NRG Suite, 1905 Benchmarks

Additional Benchmarks

		Case
PU	Thermal	PU-SOL-THERM-009 (48-inch sphere of plutonium nitrate solution)
HEU	Fast	HEU-MET-FAST-73 (Unmoderated ZEUS benchmark)
HEU	Thermal	HEU-SOL-THERM-004_case1 (Heavy water solutions, reflected spheres)
SPEC	Thermal	SPEC-MET-FAST-08 (Neptunium sphere reflected by HEU)

O.Cabellos, F.Michel-Sendis, JEFF/DOC-1843 (2017)



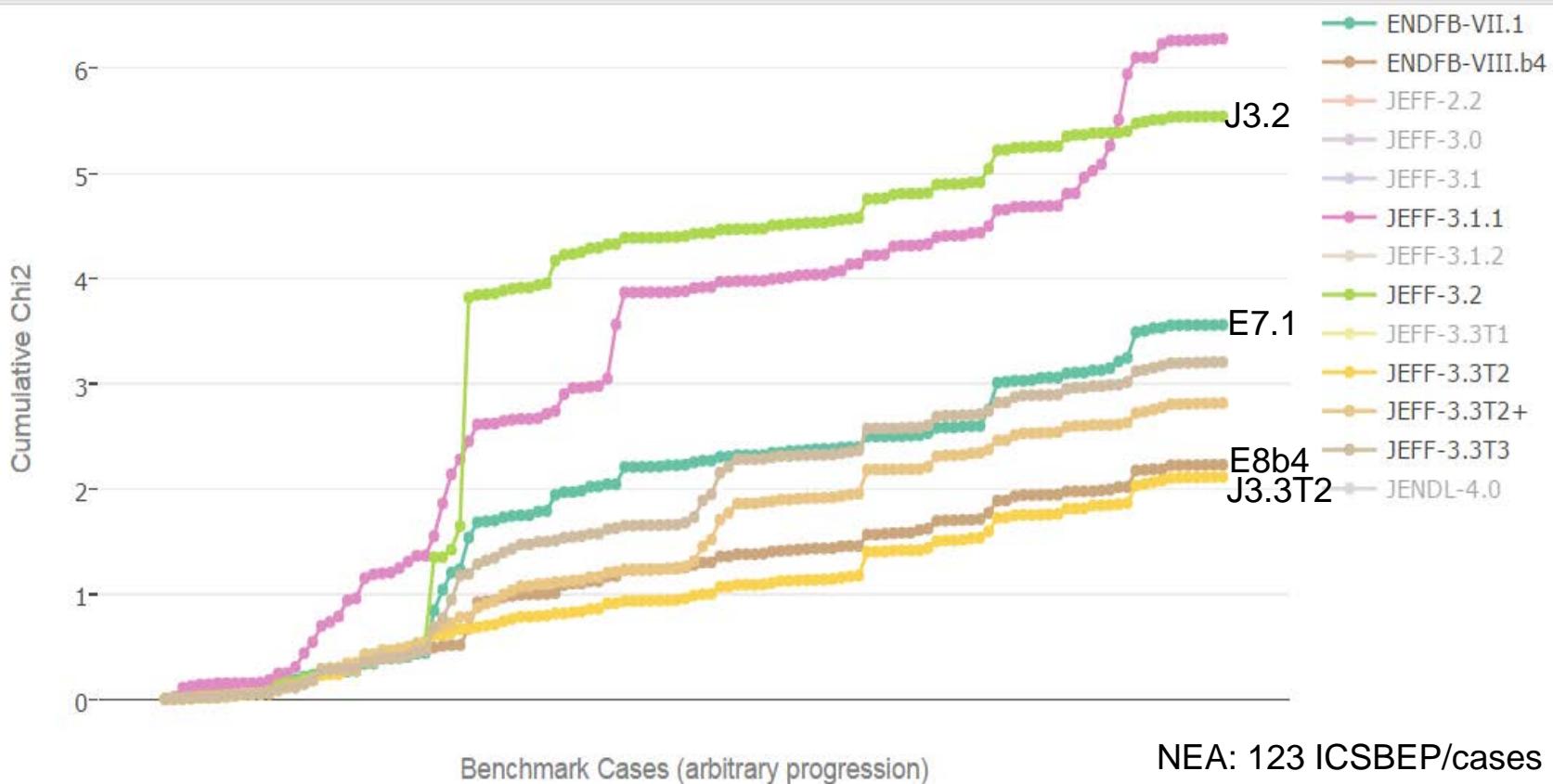
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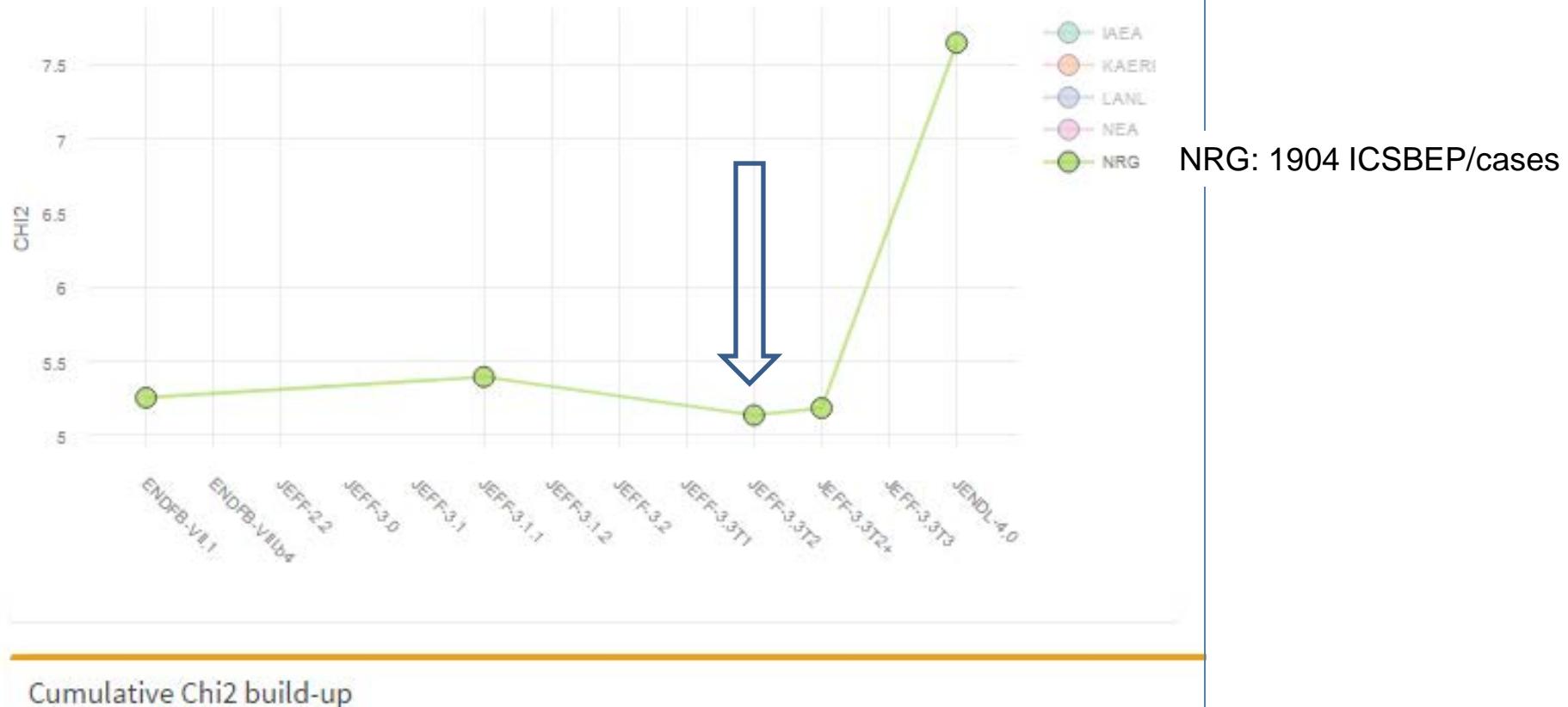


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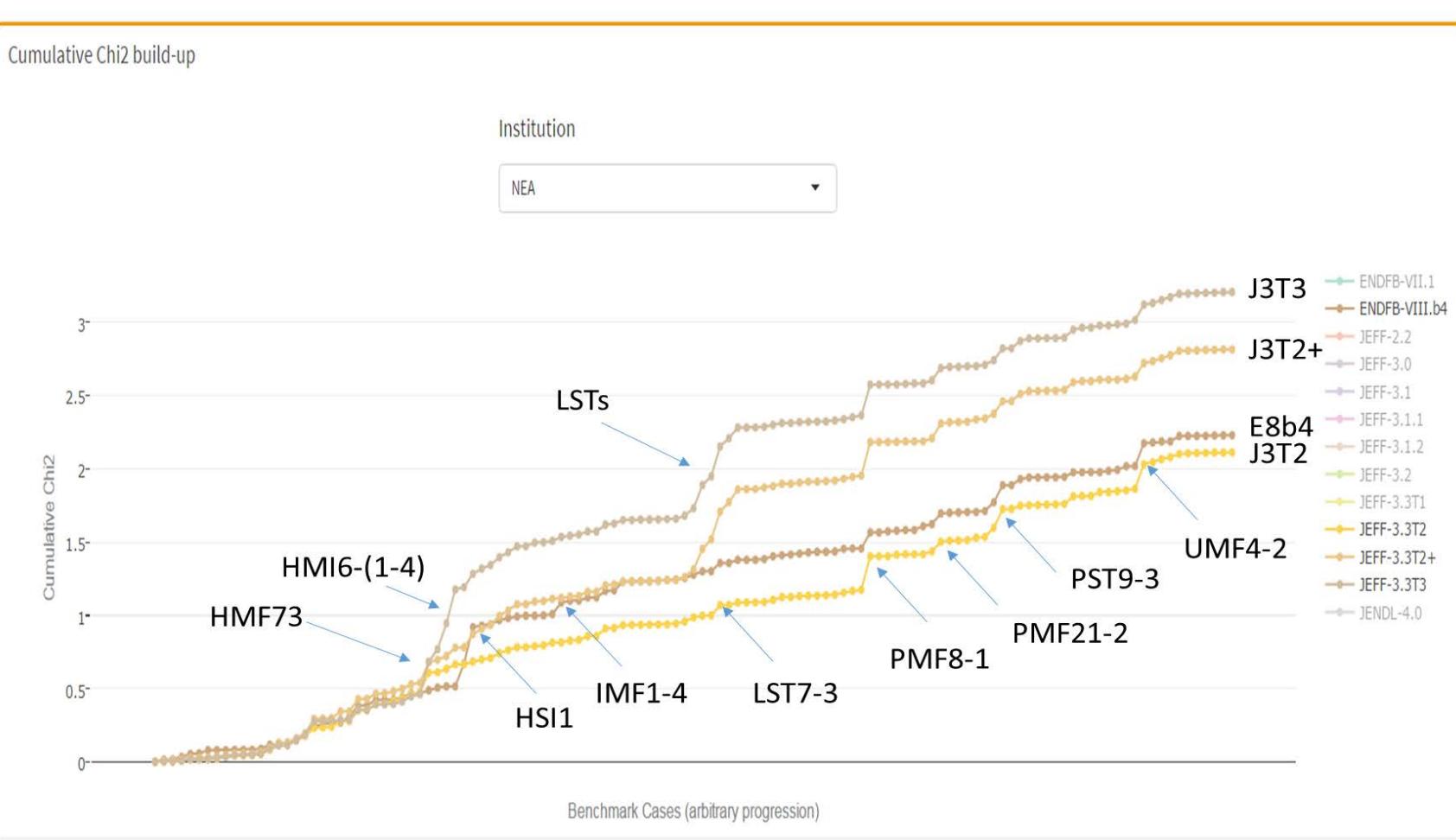
Results of criticality benchmarking using ICSBEP

Table 1. Evaluation of general performance for extended validation suites.
 Values are “*reduced*” Chi-squared, number of cases in brackets

	NEA						
	ENDF/B-VII.1	ENDF/B-VIIIb4	JEFF-3.1.1	JEFF-3.2	JEFF-3.3.T2	JEFF-3.3T2+	JEFF-3.3T3
PU	4.2 (29)	2.2 (29)	2.9 (29)	3.6 (29)	2.8 (29)	2.4 (29)	2.4 (29)
	6.1 (42)	4.1 (42)	5.3 (42)	11.8 (42)	2.2 (42)	3.5 (42)	3.9 (42)
HEU	5.0 (12)	1.9 (12)	11.3 (12)	4.9 (12)	2.7 (12)	2.1 (12)	2.2 (12)
	0.9 (13)	1.4 (13)	1.4 (13)	0.9 (13)	1.8 (13)	3.7 (13)	4.0 (13)
U233	1.7 (18)	2.1 (18)	9.5 (18)	1.2 (18)	1.7 (18)	1.9 (18)	1.7 (18)
	0.7 (8)	1.0 (8)	1.2 (8)	0.9 (8)	0.9 (8)	1.0 (8)	0.8 (8)
SPEC (C/E)	0.99249 (1)	0.99338 (1)	0.98719 (1)	0.98847 (1)	0.99142 (1)	0.99145 (1)	0.99118 (1)
Total	3.7 (123)	2.22 (123)	6.5 (123)	5.6 (123)	2.02 (123)	2.9 (123)	3.1 (123)

Results of criticality benchmarking using ICSBEP

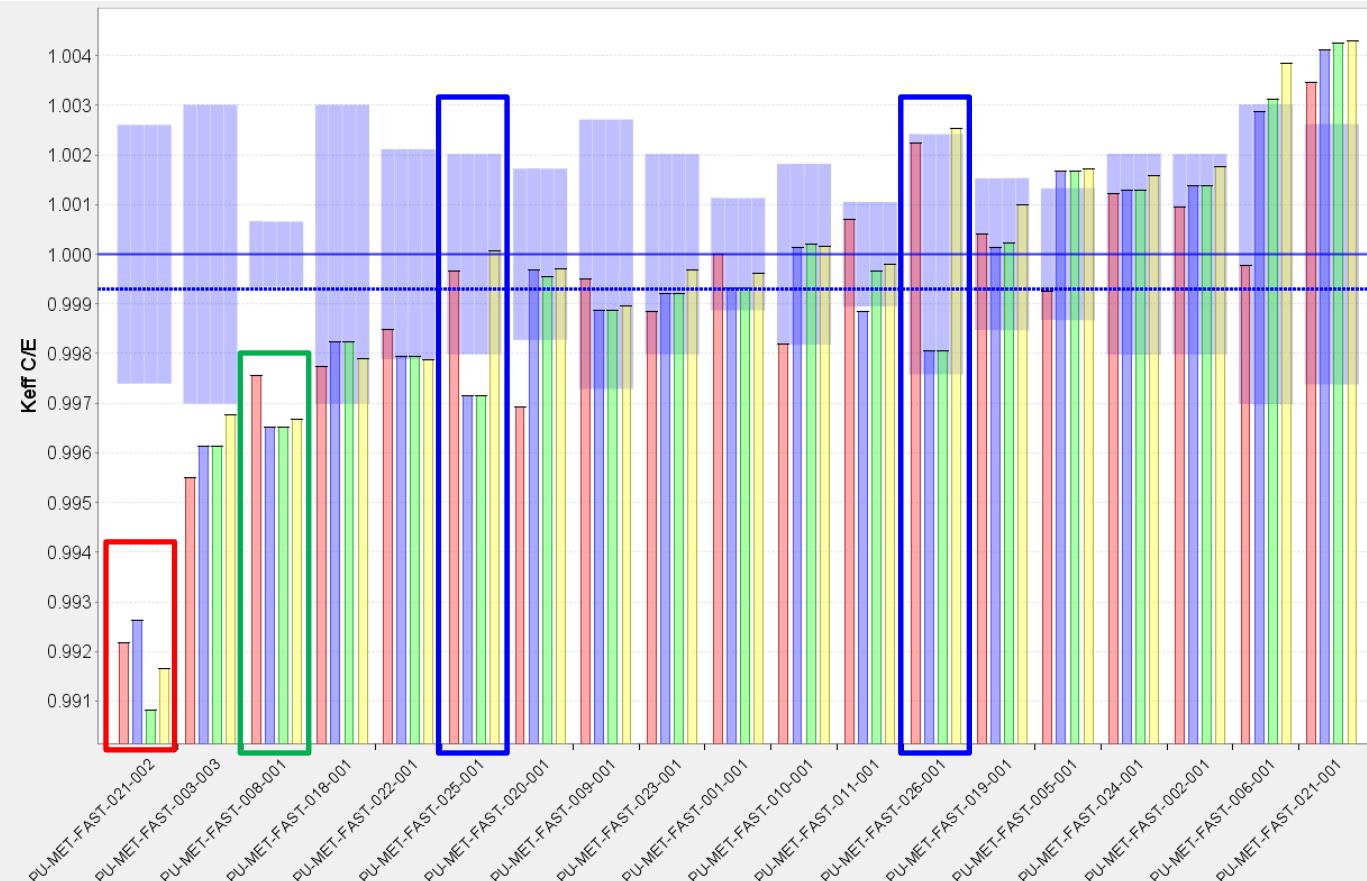
Figure 1. Cumulative Chi-2 build-up (SENDIS output)



1.1 PU-FAST

ENDF/B-VIII.b4	JEFF-3.3.T2	JEFF-3.3T2+		JEFF-3.3T3
1.5	2.2	2.4		2.6

■ NEA-ENDFB-8.b4 ■ NEA-JEFF-3.3T2 ■ NEA-JEFF-3.3T2+ ■ NEA-JEFF-3.3T3D

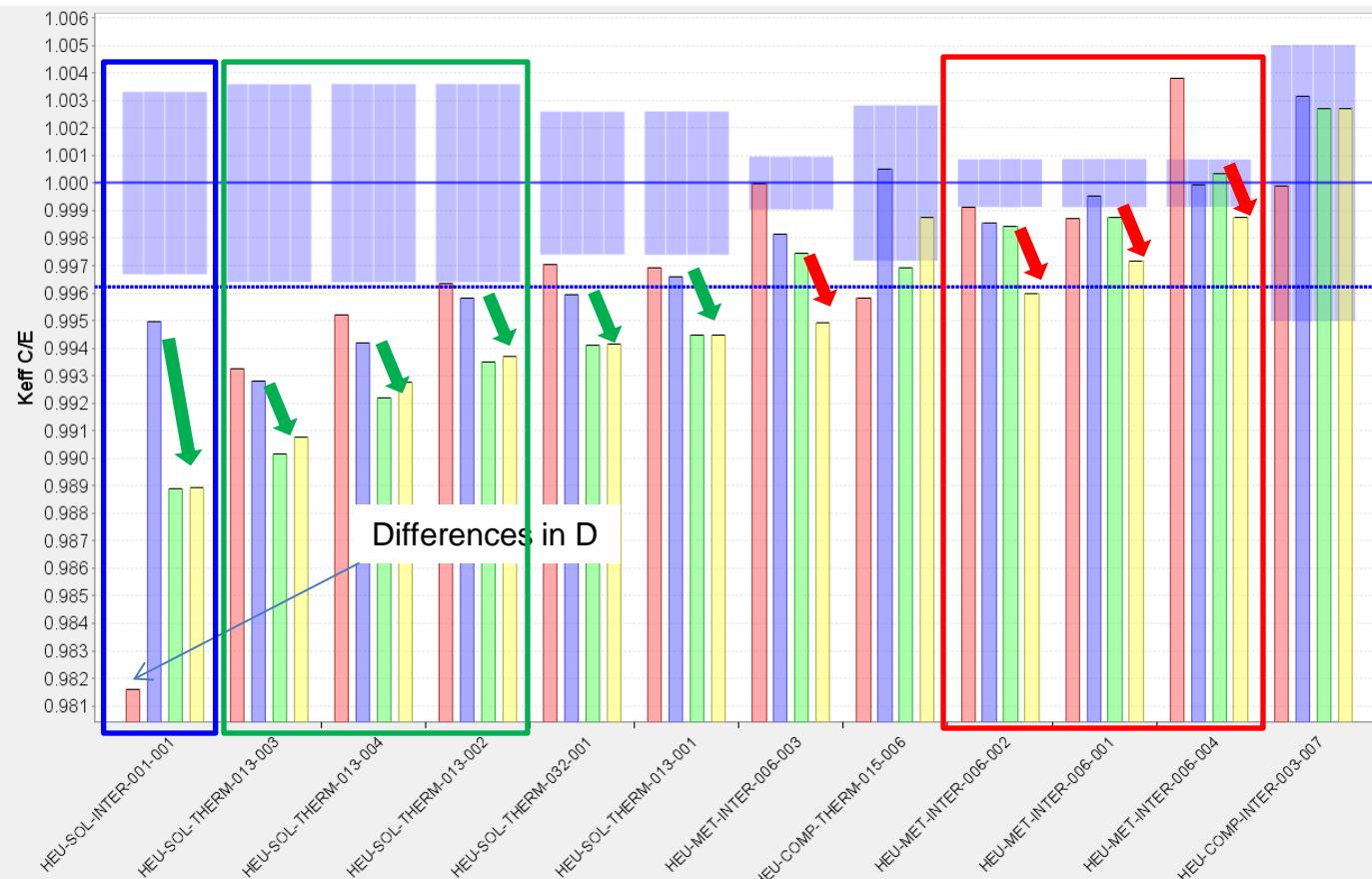


- Case with highest contribution in Chi-2
 - PMF8-1
 - PMF21-2
- JEFFvsENDFB8b4
 - PMF8-1 (Th232)
 - PMF26-1 and PMF25-1(Fe)
- JEFF
 - PMF21-2 (O16)

1.2 HEU- INTER & THERM

ENDF/B-VIII.b4	JEFF-3.3.T2	JEFF-3.3T2+		JEFF-3.3T3
12.3	2.2	6.6		3.2

■ NEA-ENDFB-8.b4
■ NEA-JEFF-3.3T2
■ NEA-JEFF-3.3T2+
■ NEA-JEFF-3.3T3D



- Case with highest contribution in Chi-2
 - HMI6-1/4

- JEFF-3.3T3
 - **HMI6-1-1(Cu)**

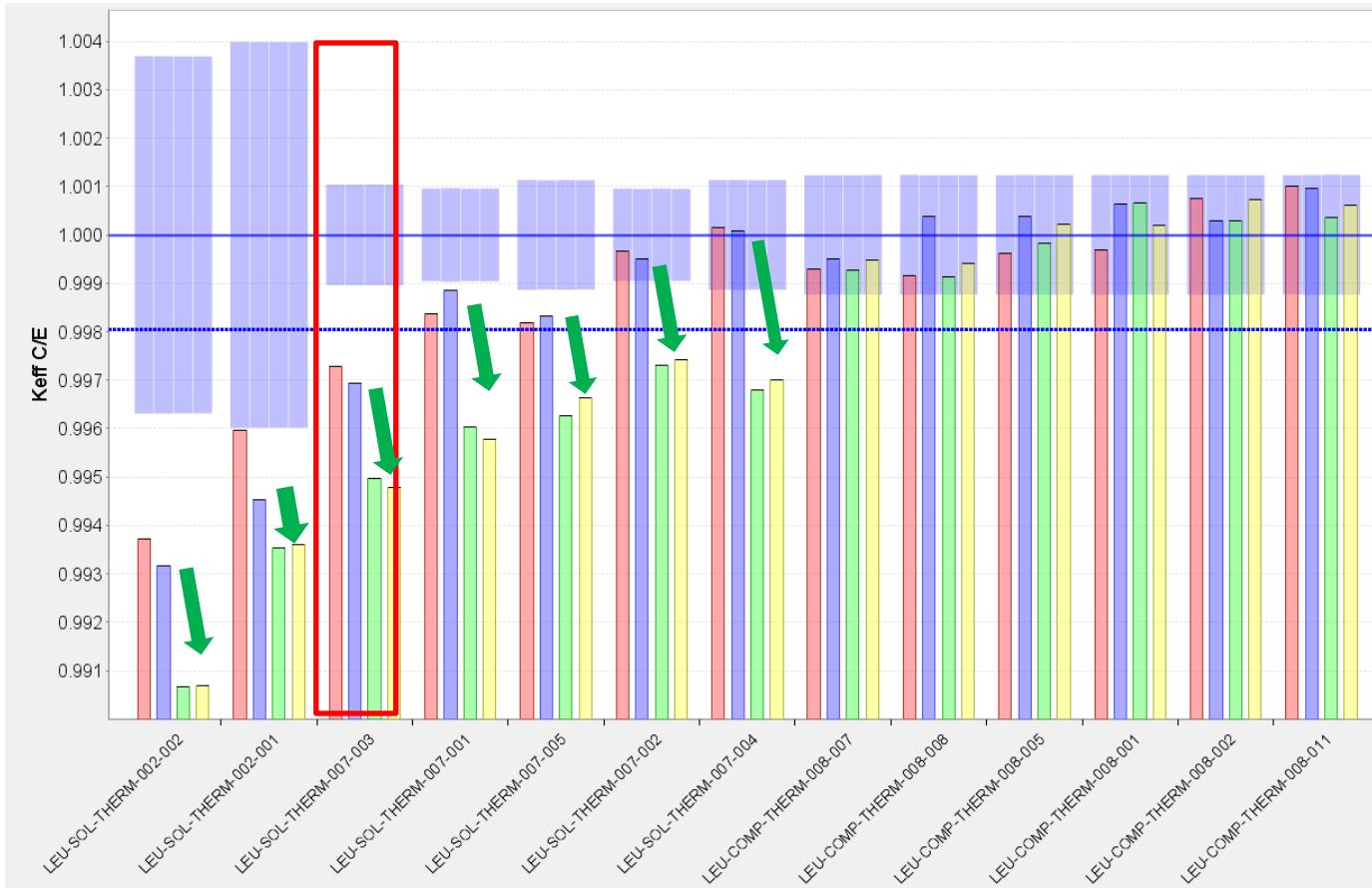
- JEFF-3.3T2vsT3
 - **HST13-1/4, HST32 and HSI1(O16&H2O)**

- ENDF/B-VIIIb4
 - **HSI1-1 (D!!!)**

1.3 LEU

ENDF/B-VIII.b4	JEFF-3.3.T2	JEFF-3.3T2+		JEFF-3.3T3
1.4	1.8	3.7		4.0

■ NEA-ENDFB-8.b4
 ■ NEA-JEFF-3.3T2
 ■ NEA-JEFF-3.3T2+
 ■ NEA-JEFF-3.3T3D



- Case with highest contribution in Chi-2
- LST7-1/5

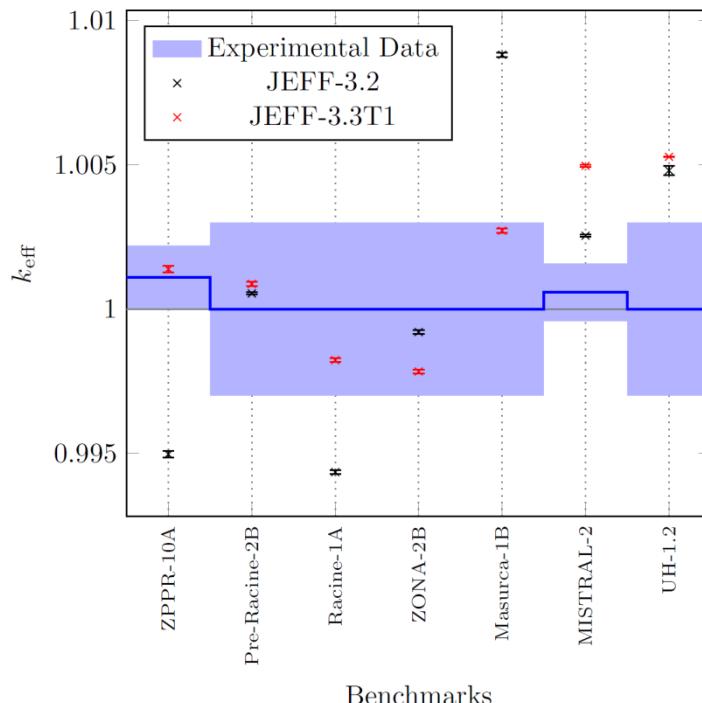
- JEFF3.3T3
- LSTs(O16&H2O)

2. Reactor benchmarks and new designs

- Validation of effective kinetics parameters (β_{eff} and Λ) based on IRPhE experiments

P. Leconte, JEF/DOC-1722 (2015)

- Experimental reactors



Experiment	$\Delta\rho(\text{JEFF33T1} - \text{JEFF32}) [\text{pcm}]$
ZPPR-10A	+644
Pre-Racine-2B	+33
Racine-1A	+391
ZONA-2B	-137
Masurca-1B	-603
Mistral-2	+240
UH1.2	+51

P. Tamagno, JEF/DOC-1752 (2016)

3. Criticality Safety - BUC Phase-VII Benchmark

“The main objective of this benchmark, is to study the ability of relevant computer codes and associated nuclear data to predict spent fuel isotopic compositions and corresponding keff values, in a cask configuration over the time duration relevant to spent nuclear fuel disposal, up to 1 000 000 years.”

Criticality calculation

O. Cabellos, JEFF/DOC-1844 (2017)

The criticality model for keff calculations is a representative cask loaded with 21 PWR-UO₂ 17×17 fuel assemblies.

Providing keff values for fresh fuel and isotopic compositions from the decay calculations (30 post-irradiation time steps, out to 1 000 000 years) for two cases involving:

- First set (ACT) of 11 actinides
- Second set (PFs) involving 14 actinides and 16 fission products

Set 1: Actinide-only burnup-credit nuclides (11 total)

²³³U, ²³⁴U, ²³⁵U, ²³⁶U, ²³⁸U, ²³⁸Pu, ²³⁹Pu, ²⁴⁰Pu, ²⁴¹Pu, ²⁴²Pu, and ²⁴¹Am

Set 2: Actinide + fission product burnup-credit nuclides (30 total)

²³³U, ²³⁴U, ²³⁵U, ²³⁶U, ²³⁸U, ²³⁷Np, ²³⁸Pu, ²³⁹Pu, ²⁴⁰Pu, ²⁴¹Pu, ²⁴²Pu, ²⁴¹Am, ^{242m}Am, ²⁴³Am, ⁹⁵Mo, ⁹⁹Tc, ¹⁰¹Ru, ¹⁰³Rh, ¹⁰⁹Ag, ¹³³Cs, ¹⁴³Nd, ¹⁴⁵Nd, ¹⁴⁷Sm, ¹⁴⁹Sm, ¹⁵⁰Sm, ¹⁵¹Sm, ¹⁵²Sm, ¹⁵¹Eu, ¹⁵³Eu, and ¹⁵⁵Gd

PWR UO₂ discharge fuel compositions for decay calculations

- 4.5-wt% 235U initial enrichment
- 50 GWd/MTU burnup

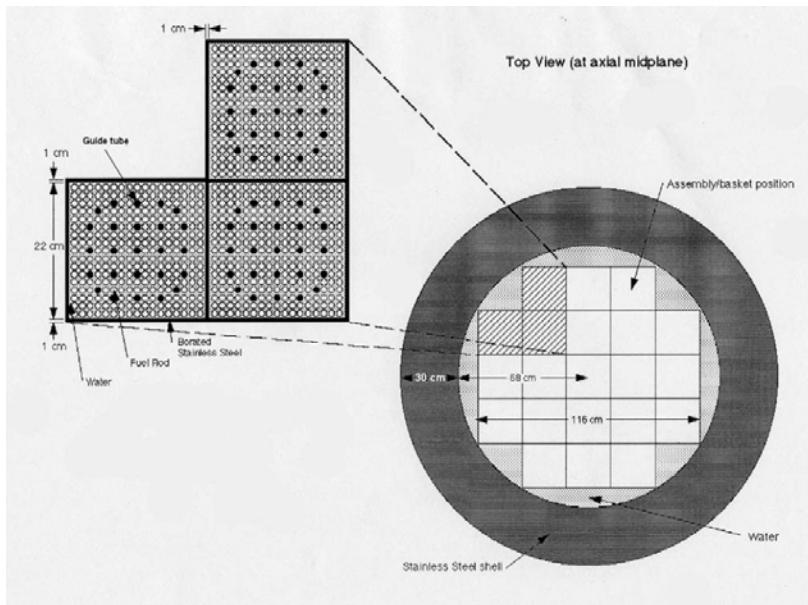


Figure. Cask model (top view)

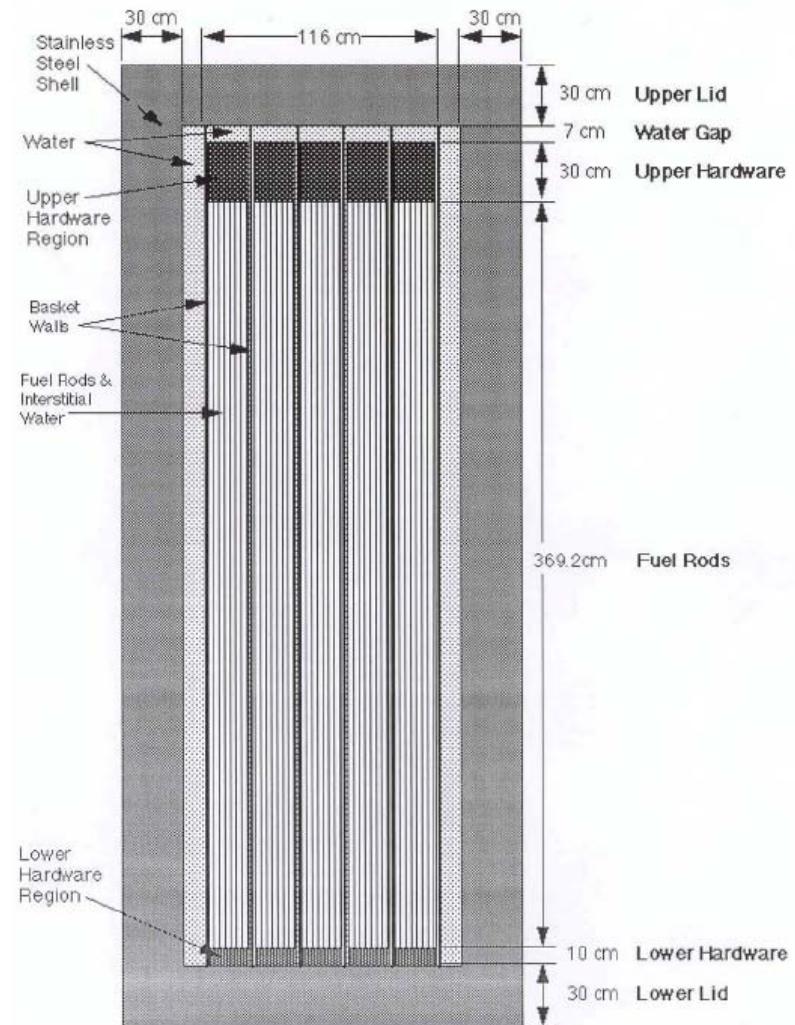
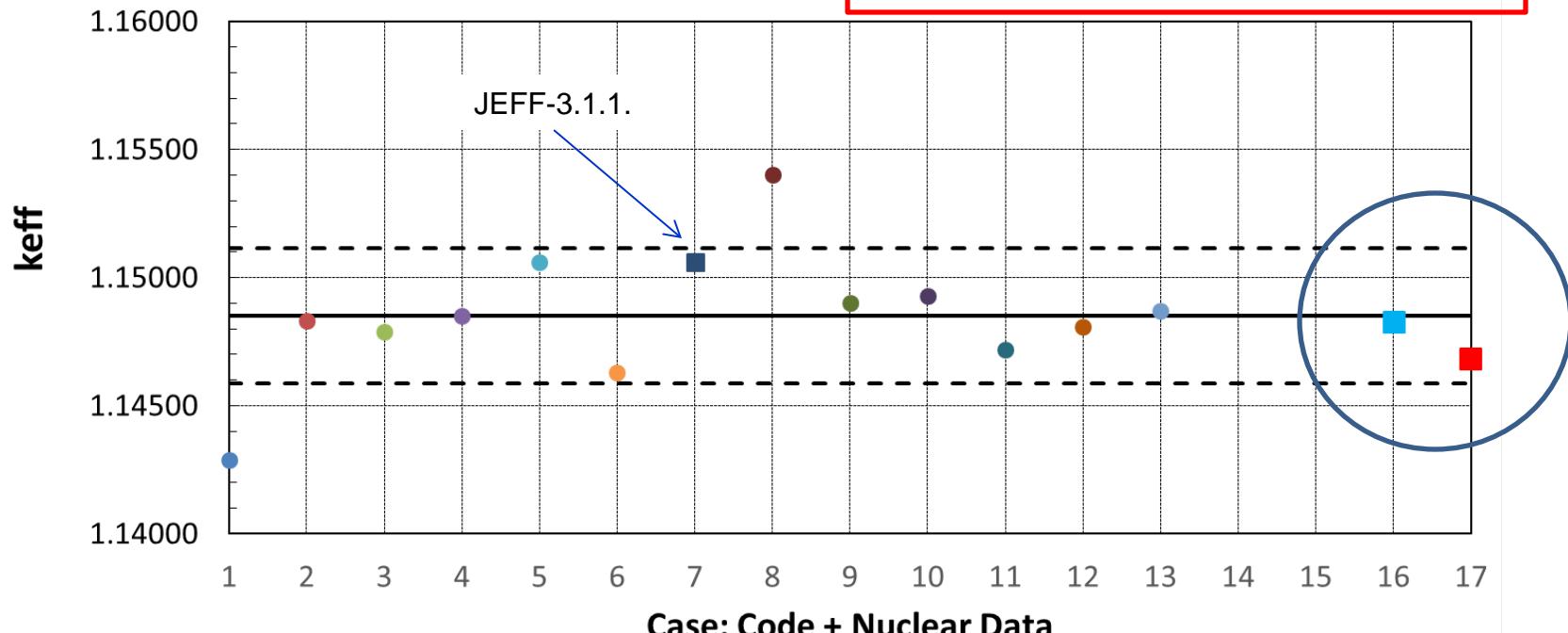
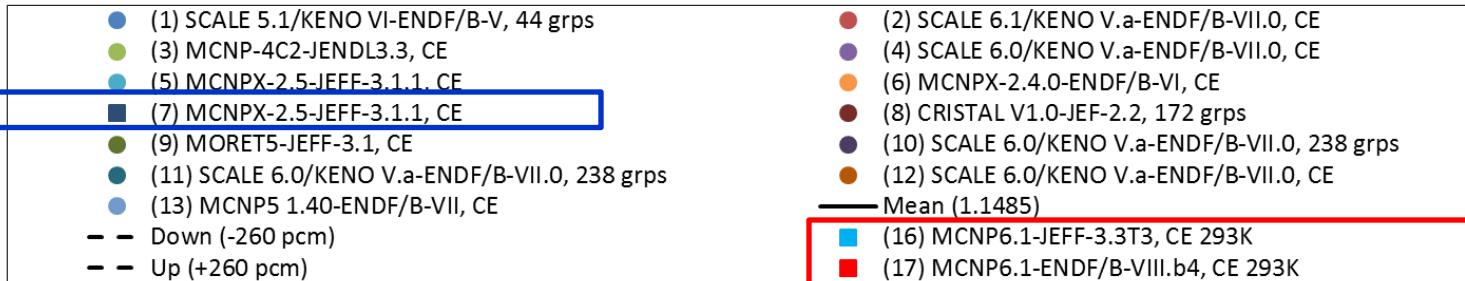


Figure. Cask model (side view)

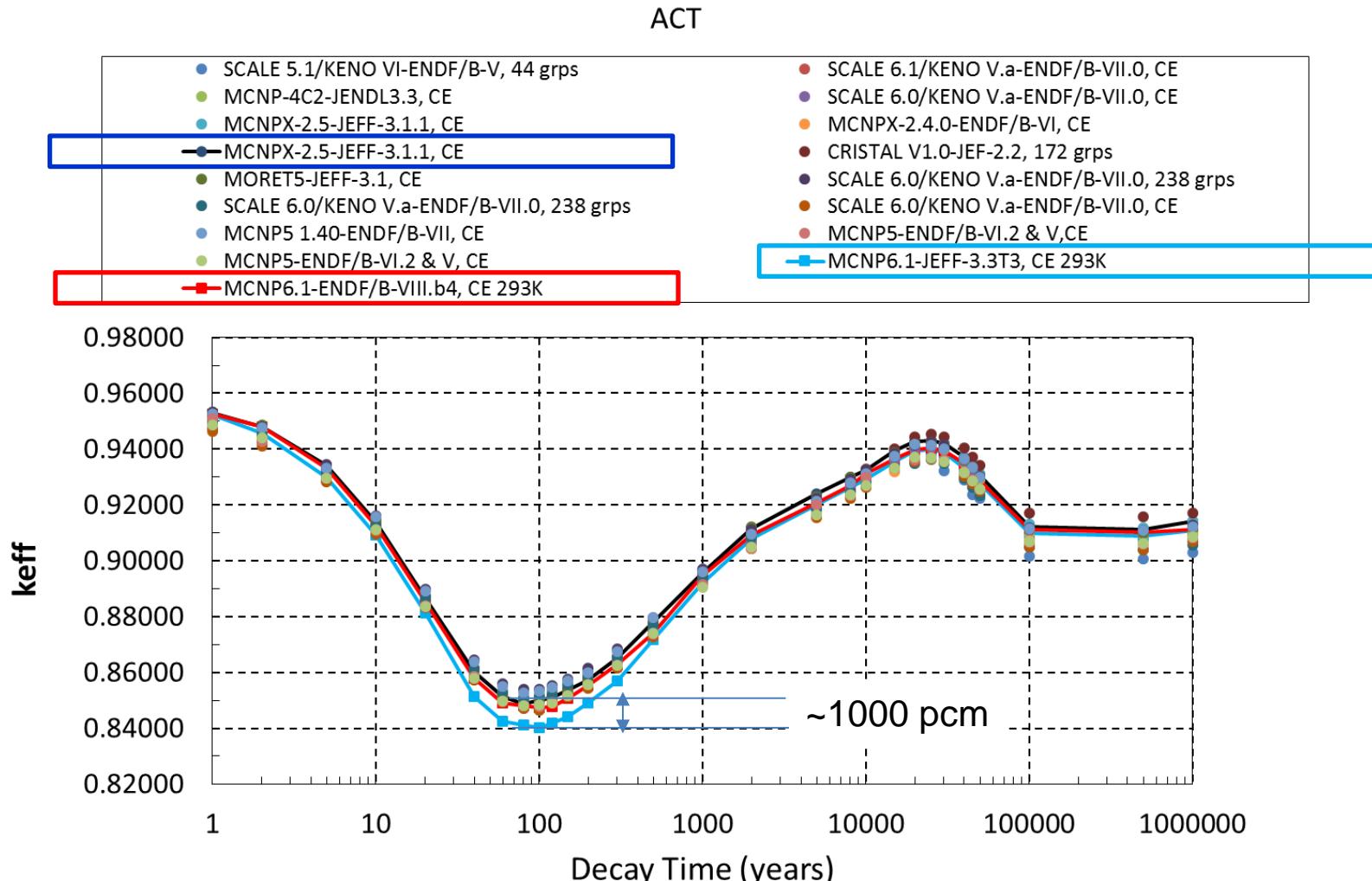
Reference: John C. Wagner and Georgeta Radulescu, Specification for Phase VII Benchmark UO₂ Fuel: Study of spent fuel compositions for long-term disposal, NEA Expert Group on Burn-up Credit, November, 2008

Keff values – mean value and std.

Keff Fresh Fuel



Keff as a function of decay time for Actinide-only in fuel



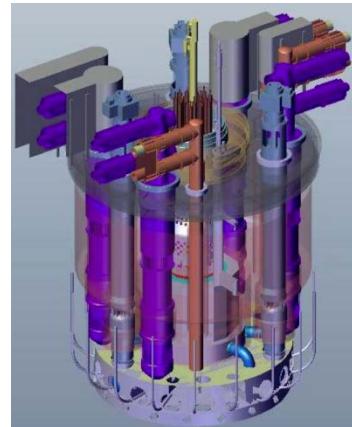
4. Reactor benchmarks and new designs

ASTRID prototype

(600 MWe)

Interm. Na circuit

Driver core ~ MOX



MOX	JEFF-3.2	JEFF-3.3T1	Diff.
k_{eff}	0.99829	1.0018	+351 pcm
Total fission probability	0.340	0.344	+1.0%
Total capture probability	0.658	0.654	-0.6%

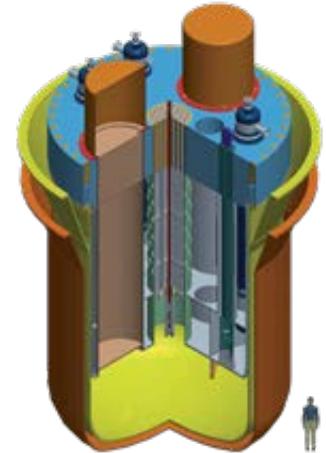
MYRRHA concept

(50-100 MWe)

Cooled by lead-bismuth I

Driver core ~ MOX

Start-up core ~ UO_2 fuel



MOX	JEFF-3.2	JEFF-3.3T1	Diff.
k_{eff}	1.00479	1.00737	+258 pcm
Total fission probability	0.343	0.346	+1.0%
Total capture probability	0.664	0.660	-0.5%
UO ₂	JEFF-3.2	JEFF-3.3T1	Diff.
k_{eff}	1.01003	1.00001	-1002 pcm
Total fission probability	0.408	0.404	-1.0%
Total capture probability	0.596	0.600	+0.7%

P. Romojaro, JEFF/DOC-1756 (2016)

5. TOF Shielding Benchmarking

Z	Material	FNS_TOF	MCNP6 Shielding Suite	Oktavian
3	Li		X	
4	Be	X	X	
6	Graphite	X	X	
7	N2	X	X	
8	O2	X		
13	Al			X
14	Si			X
22	Ti			X
24	Cr			X
25	Mn			X
26	Fe	X	X	
27	Co			X
29	Cu			X
33	As			X
34	Se			X
40	Zr			X
41	Nb			X
42	Mo			X
74	W			X
82	Pb	X	X	
92	U235, U238		X	
94	Pu239		X	

(23 elements and/or isotopes)

Compounds	FNS_TOF	MCNP6 Shielding Suite	Oktavian
Li2O	X		
Iron duct		X	
Iron duct+SS304		X	
Iron duct+SS304+PE		X	
Concrete		X	
Water		X	
LiF			X
Teflon (CF2)			X

(8 compounds/media)

K.Takise, O.Cabellos JEFF/DOC-1852 (2017)

FNS-TOF/50.0 CM(R)*5.0 CM(Z)-Iron

Angle= 0 deg	ENDF/B-VIIIb4	FENDL-3.1b	JEFF-3.3T2	JEFF-3.3T3
10 MeV < E < 16 MeV	0.95	0.95	0.95	0.95
5 MeV < E < 10 MeV	0.93	1.01	1.02	0.93
1 MeV < E < 5 MeV	0.95	0.96	0.96	0.95
0.5 MeV < E < 1 MeV	0.96	0.94	0.93	0.96
0.1 MeV < E < 0.5 MeV	1.06	1.00	1.00	1.06

Angle= 24.90 deg	ENDF/B-VIIIb4	FENDL-3.1b	JEFF-3.3T2	JEFF-3.3T3
10 MeV < E < 16 MeV	1.20	1.26	1.27	1.20
5 MeV < E < 10 MeV	0.95	0.98	1.00	0.95
1 MeV < E < 5 MeV	0.92	0.95	0.95	0.92
0.5 MeV < E < 1 MeV	1.03	0.99	1.00	1.03
0.1 MeV < E < 0.5 MeV	1.23	1.09	1.12	1.23

Angle= 41.80 deg	ENDF/B-VIIIb4	FENDL-3.1b	JEFF-3.3T2	JEFF-3.3T3
10 MeV < E < 16 MeV	0.77	0.83	0.82	0.77
5 MeV < E < 10 MeV	0.84	0.85	0.86	0.84
1 MeV < E < 5 MeV	0.89	0.91	0.91	0.89
0.5 MeV < E < 1 MeV	1.02	0.98	0.99	1.02
0.1 MeV < E < 0.5 MeV	1.20	1.07	1.09	1.20

Angle= 66.80 deg	ENDF/B-VIIIb4	FENDL-3.1b	JEFF-3.3T2	JEFF-3.3T3
10 MeV < E < 16 MeV	0.62	0.59	0.58	0.62
5 MeV < E < 10 MeV	0.74	0.74	0.75	0.74
1 MeV < E < 5 MeV	0.87	0.90	0.89	0.87
0.5 MeV < E < 1 MeV	0.95	0.91	0.91	0.95
0.1 MeV < E < 0.5 MeV	1.00	0.90	0.91	1.00

FNS-TOF/50.0 CM(R)*40.0 CM(Z)-Iron

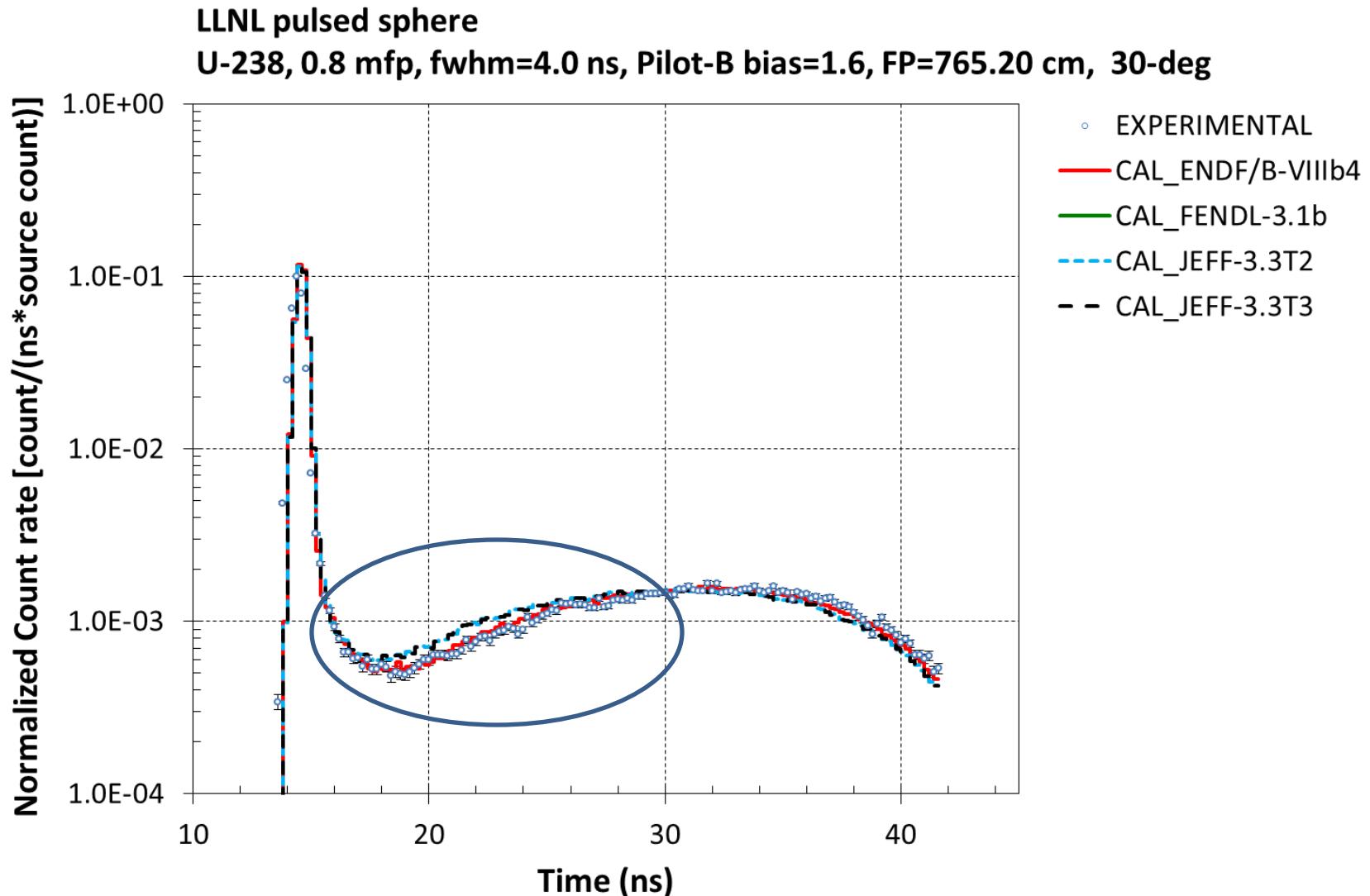
Angle= 0 deg	ENDF/B-VIIIb4	FENDL-3.1b	JEFF-3.3T2	JEFF-3.3T3
10 MeV < E < 16 MeV	0.95	0.96	0.94	0.95
5 MeV < E < 10 MeV	0.65	0.97	0.93	0.65
1 MeV < E < 5 MeV	0.96	1.15	1.08	0.96
0.5 MeV < E < 1 MeV	1.01	1.10	1.02	1.01
0.1 MeV < E < 0.5 MeV	0.96	0.94	0.93	0.96

Angle= 24.90 deg	ENDF/B-VIIIb4	FENDL-3.1b	JEFF-3.3T2	JEFF-3.3T3
10 MeV < E < 16 MeV	0.93	0.92	0.95	0.93
5 MeV < E < 10 MeV	0.80	0.97	0.94	0.80
1 MeV < E < 5 MeV	0.95	1.15	1.11	0.95
0.5 MeV < E < 1 MeV	0.98	1.07	1.01	0.98
0.1 MeV < E < 0.5 MeV	0.97	0.96	0.96	0.97

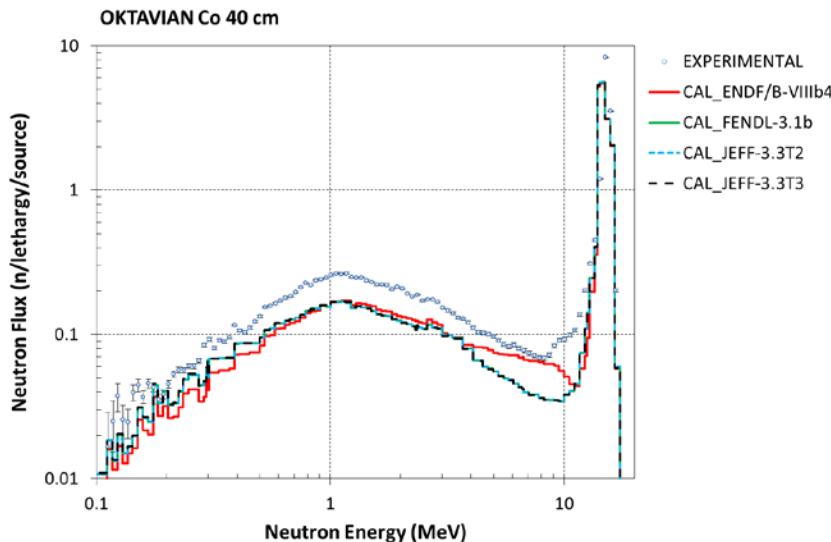
Angle= 41.80 deg	ENDF/B-VIIIb4	FENDL-3.1b	JEFF-3.3T2	JEFF-3.3T3
10 MeV < E < 16 MeV	0.86	0.81	0.87	0.86
5 MeV < E < 10 MeV	0.42	0.46	0.46	0.42
1 MeV < E < 5 MeV	0.86	1.07	1.02	0.86
0.5 MeV < E < 1 MeV	0.93	1.02	0.97	0.93
0.1 MeV < E < 0.5 MeV	0.91	0.90	0.91	0.91

Angle= 66.80 deg	ENDF/B-VIIIb4	FENDL-3.1b	JEFF-3.3T2	JEFF-3.3T3
10 MeV < E < 16 MeV	0.67	0.63	0.63	0.67
5 MeV < E < 10 MeV	0.00	0.00	0.00	0.00
1 MeV < E < 5 MeV	0.74	0.94	0.88	0.74
0.5 MeV < E < 1 MeV	0.87	0.97	0.92	0.87
0.1 MeV < E < 0.5 MeV	0.84	0.82	0.85	0.84

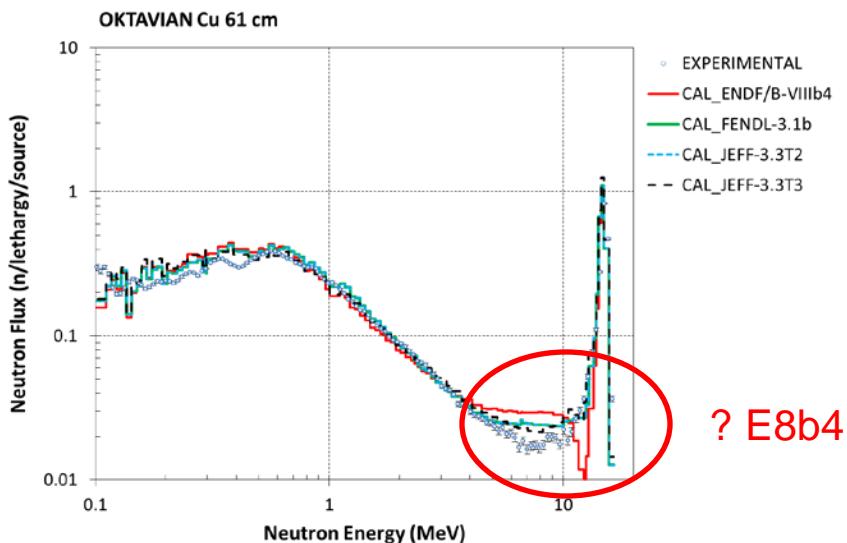
□ U238, overestimation 18-26 ns



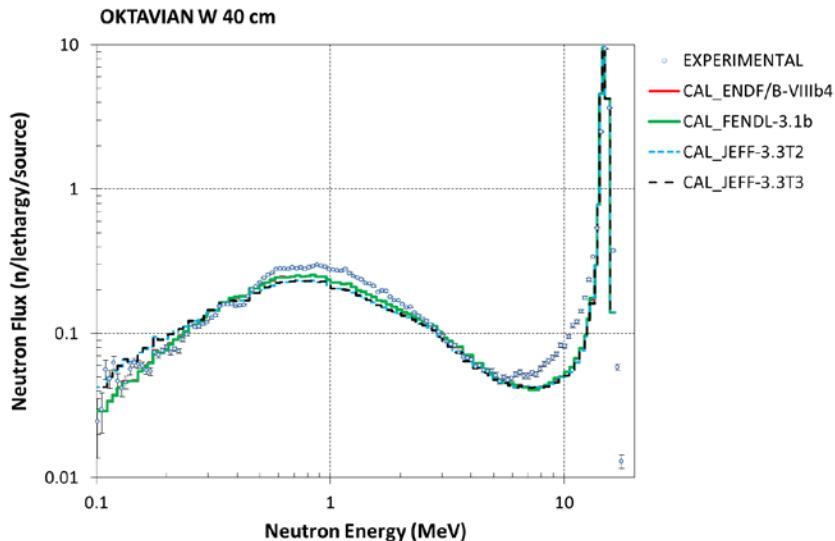
☐ Co, all libraries high underestimation



☐ Cu, slightly better T2=FENDL-3.1b



☐ W, T2/T3 lower values below 1 MeV



☐ Zr, JEFF/3.3T3 better agreement

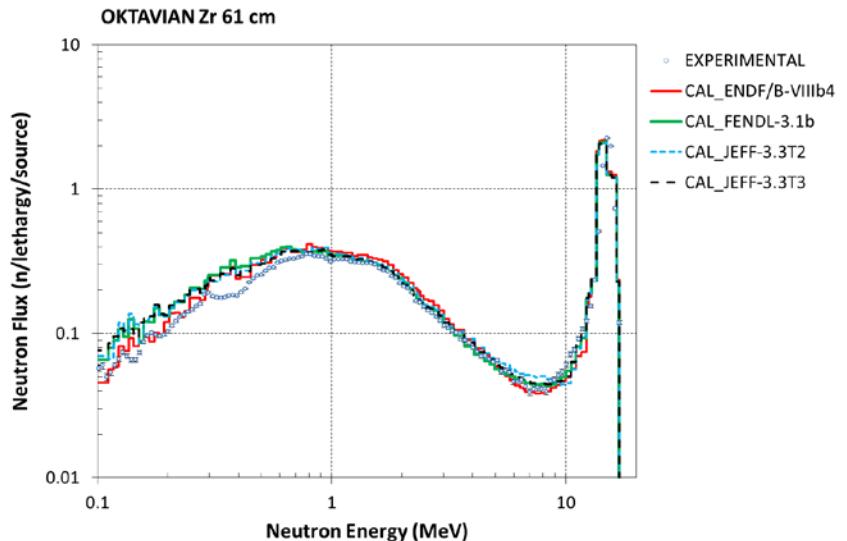


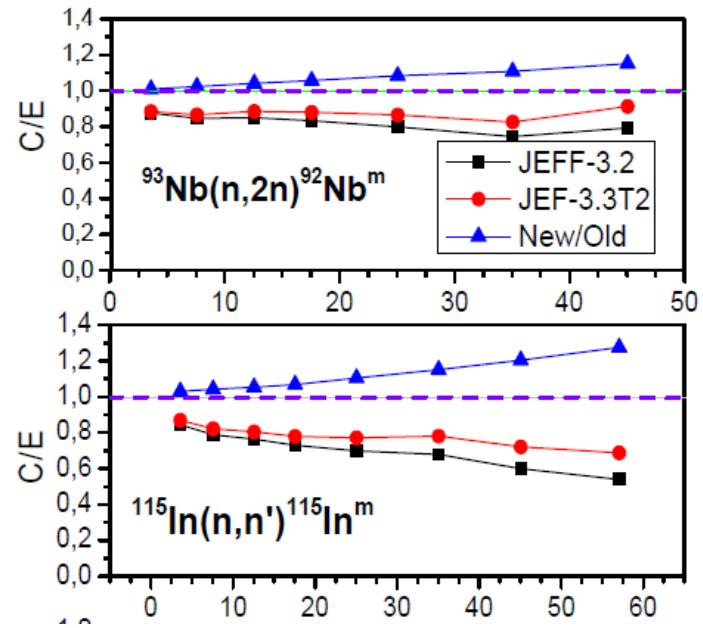
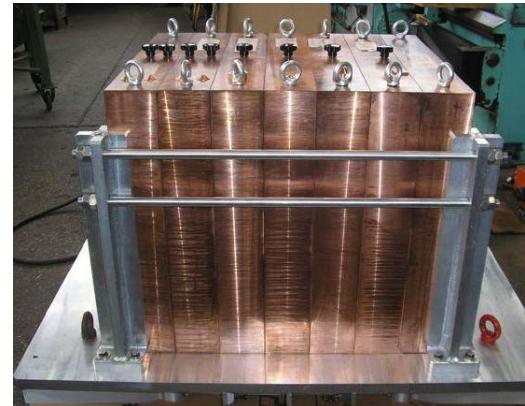
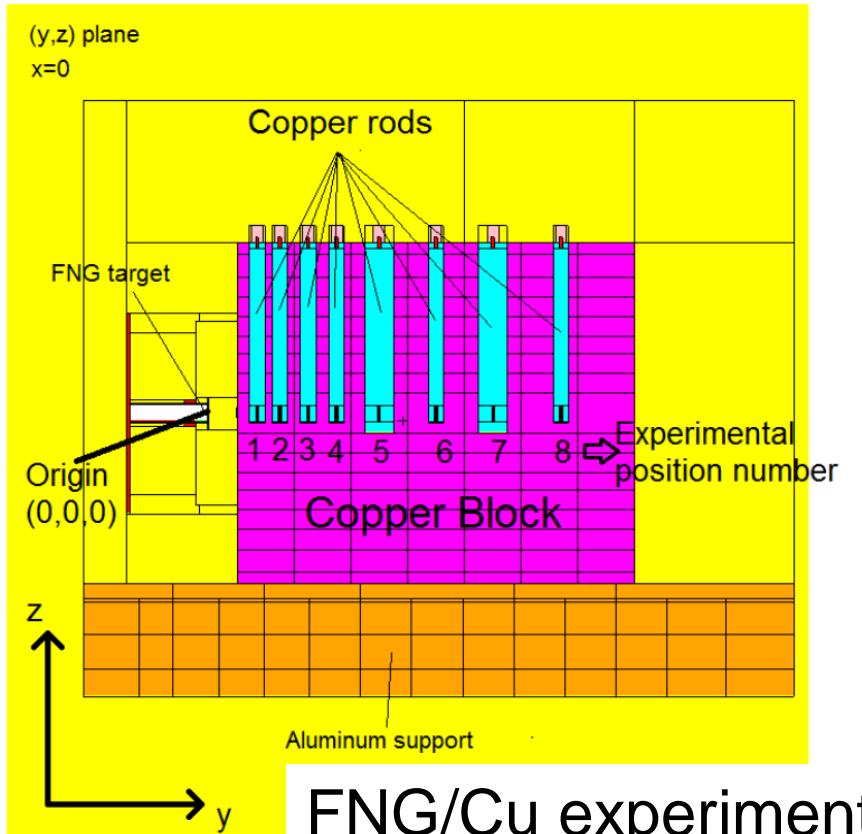
Table. <C>/<E> values

	ENDF/B-VIIIb4	FENDL-3.1b	JEFF-3.3T2	JEFF-3.3T3		ENDF/B-VIIIb4	FENDL-3.1b	JEFF-3.3T2	JEFF-3.3T3	
Oktavian Al-40 cm						Oktavian As-40 cm				
10 MeV < E < 16 MeV	1.01	1.01	1.01	1.01		0.82	-	0.83	0.83	
5 MeV < E < 10 MeV	0.91	0.90	0.90	0.90		0.88	-	0.92	0.92	
1 MeV < E < 5 MeV	0.91	0.91	0.91	0.91		1.22	-	1.14	1.14	
0.5 MeV < E < 1 MeV	0.93	0.93	0.93	0.94		1.12	-	1.08	1.08	
0.1 MeV < E < 0.5 MeV	1.41	1.38	1.38	1.41		1.23	-	1.27	1.27	
Oktavian Co-40 cm						Oktavian Cr-40cm				
10 MeV < E < 16 MeV	0.81	0.83	0.83	0.83		0.92	0.93	0.93	0.93	
5 MeV < E < 10 MeV	0.89	0.55	0.55	0.55		1.18	1.06	1.07	1.07	
1 MeV < E < 5 MeV	0.69	0.64	0.64	0.64		1.17	1.12	1.14	1.14	
0.5 MeV < E < 1 MeV	0.58	0.61	0.61	0.62		1.15	1.25	1.23	1.23	
0.1 MeV < E < 0.5 MeV	0.64	0.77	0.77	0.78		1.16	1.07	1.05	1.05	
Oktavian Cu-61cm						Oktavian LiF-61 cm				
10 MeV < E < 16 MeV	0.91	1.02	1.02	1.15		1.05	1.05	1.05	1.05	
5 MeV < E < 10 MeV	1.58	1.31	1.31	1.28		0.87	0.88	0.88	0.87	
1 MeV < E < 5 MeV	1.01	1.12	1.12	1.07		0.88	0.88	0.88	0.88	
0.5 MeV < E < 1 MeV	0.99	1.01	1.01	0.93		0.67	0.65	0.67	0.67	
0.1 MeV < E < 0.5 MeV	1.15	1.11	1.11	1.16		0.85	0.82	0.85	0.85	

Table. <C>/<E> values

	ENDF/B-VIIIb4	FENDL-3.1b	JEFF-3.3T2	JEFF-3.3T3		ENDF/B-VIIIb4	FENDL-3.1b	JEFF-3.3T2	JEFF-3.3T3	
Oktavian Ti-40cm						Oktavian W-40cm				
10 MeV < E < 16 MeV	0.93	0.93	0.93	0.93		0.87	0.87	0.88	0.88	
5 MeV < E < 10 MeV	1.26	1.25	1.18	1.18		0.81	0.81	0.80	0.80	
1 MeV < E < 5 MeV	1.28	1.28	1.26	1.26		0.94	0.94	0.87	0.87	
0.5 MeV < E < 1 MeV	1.24	1.25	1.22	1.22		0.81	0.81	0.74	0.74	
0.1 MeV < E < 0.5 MeV	1.69	1.67	1.66	1.68		1.07	1.06	1.13	1.13	
<hr/>										
Oktavian Zr-40cm										
10 MeV < E < 16 MeV	0.97	0.94	0.93	0.94						
5 MeV < E < 10 MeV	0.96	1.03	1.12	1.05						
1 MeV < E < 5 MeV	1.19	1.09	1.13	1.10						
0.5 MeV < E < 1 MeV	1.07	1.06	1.06	1.03						
0.1 MeV < E < 0.5 MeV	1.23	1.44	1.37	1.38						

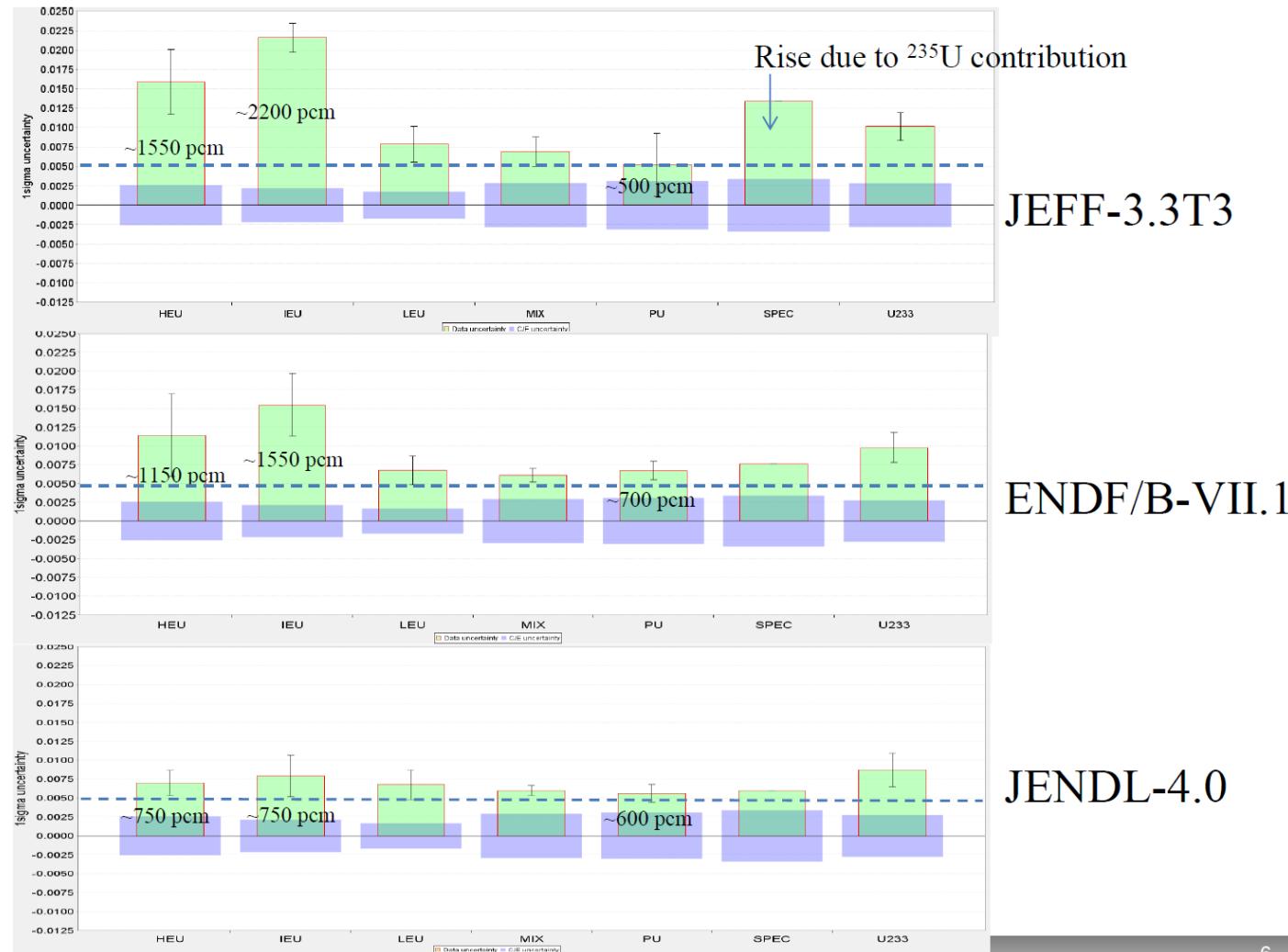
6. Shielding and fusion application



M. Angelone,
EFF/DOC-1808(2016)

7. Covariance verification

- **NDaST**
- S/U Propagation
of only XS uncert.
- and
- comparison
- with
- Exp. Uncertainties



8. Conclusion

- Importance of Joint Evaluation: U5/8-Pu9-1H-16O
 - JEFF-3.3 T3 -> T2
- Compensation effects cross-sections and angular distributions
 - Cu63/65
- Covariances in U5/U8-Pu9
 - Large impact in criticality ICSBEP benchmarks
 - No-tuning with integral benchmarks (U5/U8-Pu9 in JEFF-3.3 T3)
- Benchmarking and Validation
 - Criticality (ICSBEP), Shielding (TOF, Fusion,...)
 - New designs: MYRRHA, ASTRID, ALFRED, ...
 - Customers: WPCNS-new data for Ice-water,...
- New tools for visualization/analysis
 - Populate DICE database with around 14000 C/E values ...
 - Figure of Merit, trends www.sendis.org