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Data uncertainty analysis for the proposed benchmark exercise using ERANOS in conjunction with unadjusted libraries, i.e. JEFF-3.1/BOLNA and JEF-2.2, as well as with the adjusted library ERALIB-1

Methodology

Deterministic ERANOS in conjunction with these basic/covariance data sets:

•JEFF-3.1/BOLNA (unadjusted), with Version 2.2.
BOLNA: **B**rookhaven, **O**ak Ridge, **L**os Alamos, **N**RG and **A**rgonne.

•JEF-2.2/JEF-2.2 (unadjusted), i.e. JEF-2.2, with Version 2.2.

•ERALIB-1/ERALIB-1 (adjusted), i.e. ERALIB1, with Version 2.1.
ERALIB-1: Eric Fort, adjustment made with respect to several sodium-cooled fast spectrum system experiments.

As requested: 33 group discrete-ordinates transport-theory (BISTRO for cylindrical geometry) with P_1S_4 approximations (symmetric weight set) + given correction factors.
Same meshing as in the benchmark specifications (not given for the ABR core: Input preparation is complex and time consuming).

Sensitivity coefficients: Perturbation theory for k_{eff} ($|k_{eff} - k_{eff}\ adj| < 0.0001$);
Generalized perturbation theory for reaction rate ratios at core center;
Extended perturbation theory for reactivity effects.

JEZEBEL-Pu239

JEZEBEL-Pu239/ Library	Calculated parameter	Corrected calculated parameter	1σ-uncertainty (%)	Experiment /1σ-uncertainty (%)
k_{eff}				
JEFF-3.1/BOLNA	1.00493	0.99941	0.417	1.00000/0.2
JEF-2.2	1.00163	0.99613	2.34	
ERALIB1	1.00767	1.00214	0.35	
F28/F25 (at core center)				
JEFF-3.1/BOLNA	0.204	0.210	2.45	0.214/1.1
JEF-2.2	0.199	0.204	2.55	
ERALIB1	0.196	0.201	0.98	
F37/F25 (at core center)				
JEFF-3.1/BOLNA	0.975	0.984	6.68	0.962/1.4
JEF-2.2	0.914	0.922	9.01	
ERALIB1	0.916	0.924	8.87	
F49/F25 (at core center)				
JEFF-3.1/BOLNA	1.436	1.439	0.72	1.448/0.9
JEF-2.2	1.429	1.432	3.53	
ERALIB1	1.440	1.443	0.70	

In red: No common range between experimental and calculational values by accounting for their uncertainties.

JEZEBEL-Pu239 (continued)

Most important contributions to the data uncertainty of k_{eff}:
JEFF-3.1/BOLNA: Pu239 fission: 0.3%.
JEF-2.2: *Pu239 fission*: 2.3%.
ERALIB1: Pu239 fission: 0.3%.

Most important contributions to the data uncertainty of F28/F25:
JEFF-3.1/BOLNA: Pu239 inelastic scattering: 2.5% (*neither U238 fission nor U235 fission*).
JEF-2.2: U238 fission: 1.6%; U235 fission: 1.4%; Pu239 inelastic scattering: 1.4%.
ERALIB1: Pu239 inelastic scattering: 0.8% (*neither U238 fission nor U235 fission*).

Most important contributions to the data uncertainty of F37/F25:
JEFF-3.1/BOLNA: Np237 fission: 6.5%; Pu239 inelastic scattering: 1.6%.
JEF-2.2: Np237 fission: 8.8%; U235 fission: 1.4%; Pu239 inelastic scattering: 1.0%.
ERALIB1: Np237 fission: 8.8%.

Most important contributions to the data uncertainty of F49/F25:
JEFF-3.1/BOLNA: Pu239 fission: 0.5%; U235 fission: 0.4%; Pu239 inelastic scattering: 0.4%.
JEF-2.2: Pu239 fission: 3.3%; U235 fission: 1.1%.
ERALIB1: Pu239 fission: 0.5%; U235 fission: 0.5%.

JEZEBEL-Pu240

JEZEBEL-Pu240/ Library	Calculated parameter	Corrected calculated parameter	1σ-uncertainty (%)	Experiment /1σ-uncertainty (%)
k_{eff}				
JEFF-3.1/BOLNA	1.00851	1.00374	0.667	1.00000/0.2
JEF-2.2	1.00399	0.99924	2.108	
ERALIB1	1.01062	1.00584	0.344	

Most important contributions to the data uncertainty of k_{eff}:

JEFF-3.1/BOLNA: A variety of reactions of the Pu isotopes.

JEF-2.2: *Pu239 fission*: 1.9%.

ERALIB1: A variety of reactions of the Pu isotopes.

FLATTOP-Pu239

FLATTOP-Pu239/ Library	Calculated parameter	Corrected calculated parameter	1σ-uncertainty (%)	Experiment /1σ-uncertainty (%)
k_{eff}				
JEFF-3.1/BOLNA	0.99794	0.99929	0.711	1.00000/0.3
JEF-2.2	0.98089	0.98222	2.107	
ERALIB1	0.99323	0.99457	0.252	
F28/F25 (at core center)				
JEFF-3.1/BOLNA	0.1722	0.1774	1.95	0.1799/1.1
JEF-2.2	0.1710	0.1762	2.40	
ERALIB1	0.1681	0.1732	0.87	
F37/F25 (at core center)				
JEFF-3.1/BOLNA	0.8549	0.8621	6.60	0.8561/1.4
JEF-2.2	0.8098	0.8166	9.01	
ERALIB1	0.8090	0.8158	8.89	

FLATTOP-Pu239 (continued)

Most important contributions to the data uncertainty of k_{eff}:
JEFF-3.1/BOLNA: *U238 inelastic scattering*: 0.6%.
JEF-2.2: *Pu239 fission*: 2.0%.
ERALIB1: Pu239 fission: 0.2%.

Most important contributions to the data uncertainty of F28/F25:
JEFF-3.1/BOLNA: Pu239 inelastic scattering: 1.8% (*neither U238 fission nor U235 fission*).
JEF-2.2: U238 fission: 1.6%; U235 fission: 1.4%; Pu239 inelastic scattering: 1.0%.
ERALIB1: U238 fission: 0.6%; Pu239 inelastic scattering: 0.5%.

Most important contributions to the data uncertainty of F37/F25:
JEFF-3.1/BOLNA: Np237 fission: 6.4%; Pu239 inelastic scattering: 1.2%.
JEF-2.2: Np237 fission: 8.9%; U235 fission: 1.4%.
ERALIB1: Np237 fission: 8.9%.

ZPR-6 Assembly 7

ZPR-6 Assembly 7/ Library	Calculated parameter	Corrected calculated parameter	1σ-uncertainty (%)	Experiment /1σ-uncertainty (%)
k_{eff}				
JEFF-3.1/BOLNA	0.99015	1.00195	1.178	1.00051/0.23
JEF-2.2	0.98274	0.99446	1.595	
ERALIB1	0.99060	1.00241	0.144	
F49/F25 (at core center)				
JEFF-3.1/BOLNA	0.9190	0.9051	0.86	0.9435/2.1
JEF-2.2	0.9183	0.9044	2.52	
ERALIB1	0.9357	0.9216	0.38	
F28/F25 (at core center)				
JEFF-3.1/BOLNA	0.0218	0.0224	6.54	0.0233/3.0
JEF-2.2	0.0224	0.0230	3.76	
ERALIB1	0.0224	0.0230	0.57	
C28/F25 (at core center)				
JEFF-3.1/BOLNA	0.1380	0.1329	2.18	0.1323/2.4
JEF-2.2	0.1390	0.1339	1.53	
ERALIB1	0.1388	0.1337	0.41	

ZPR-6 Assembly 7 (continued)

Most important contributions to the data uncertainty of k_{eff}:
JEFF-3.1/BOLNA: *U238 inelastic scattering*: 0.8%; U238 capture: 0.5%.
JEF-2.2: *Pu239 fission*: 1.3%.
ERALIB1: Pu239 fission: 0.1%.

Most important contributions to the data uncertainty of F49/F25:
JEFF-3.1/BOLNA:U235 fission: 0.5%; Pu239 fission: 0.4%; U238 capture: 0.2%.
JEF-2.2: Pu239 fission: 2.3%.
ERALIB1: Pu239 fission: 0.3%.

Most important contributions to the data uncertainty of F28/F25:
JEFF-3.1/BOLNA: U238 inelastic scattering: 6.1% (*neither U238 fission nor U235 fission*).
JEF-2.2: Na inelastic scattering: 2.1%; U238 inelastic scattering: 1.8%; U238 fission: 1.5%; Fe56 inelastic scattering: 1.1%.
ERALIB1: Various isotopes and reactions.

Most important contributions to the data uncertainty of C28/F25:
JEFF-3.1/BOLNA: U238 capture: 2.1%.
JEF-2.2: U238 capture: 1.1%; U235 fission: 1.0%.
ERALIB1: U238 capture: 0.3%; U235 fission: 0.2%.

ZPR-6 Assembly 7 High Pu240

ZPR-6 Assembly 7 High Pu240/ Library	Calculated parameter	Corrected calculated parameter	1σ-uncertainty (%)	Experiment /1σ-uncertainty (%)
k_{eff}				
JEFF-3.1/BOLNA	0.98933	1.00171	1.192	1.00080/0.220
JEF-2.2	0.98123	0.99350	1.576	
ERALIB1	0.98917	1.00154	0.141	

Most important contributions to the data uncertainty of k_{eff}:
JEFF-3.1/BOLNA: *U238 inelastic scattering*: 0.9%; U238 capture: 0.5%.
JEF-2.2: *Pu239 fission*: 1.3%.
ERALIB1: Pu239 fission: 0.1%.

ZPPR-9

ZPPR-9/ Library	Calculated parameter	Corrected calculated parameter	1σ-uncertainty (%)	Experiment /1σ-uncertainty (%)
k_{eff}				
JEFF-3.1/BOLNA	0.98882	0.99678	1.379	1.00080/0.154
JEF-2.2	0.98327	0.99119	1.622	
ERALIB1	0.99119	0.99917	0.144	
F28/F25 (at core center)				
JEFF-3.1/BOLNA	0.01959	0.02076	7.80	0.02210/2.76
JEF-2.2	0.02049	0.02172	3.73	
ERALIB1	0.02039	0.02162	0.52	
F49/F25 (at core center)				
JEFF-3.1/BOLNA	0.9095	0.9031	0.89	0.9295/1.99
JEF-2.2	0.9099	0.9035	2.49	
ERALIB1	0.9257	0.9193	0.38	
C28/F25 (at core center)				
JEFF-3.1/BOLNA	0.1364	0.1387	2.25	0.1379/1.89
JEF-2.2	0.1373	0.1397	1.53	
ERALIB1	0.1374	0.1397	0.40	

ZPPR-9 (continued)

Most important contributions to the data uncertainty of k_{eff}:
JEFF-3.1/BOLNA: *U238 inelastic scattering*: 1.1%; U238 capture: 0.6%.
JEF-2.2: *Pu239 fission*: 1.3%.
ERALIB1: Pu239 fission: 0.1%.

Most important contributions to the data uncertainty of F28/F25:
JEFF-3.1/BOLNA: U238 inelastic scattering: 7.5%; O16 elastic scattering: 1.3%; Fe56 inelastic scattering: 0.9% (*neither U238 fission nor U235 fission*).
JEF-2.2: U238 inelastic scattering: 2.3%; Na23 inelastic scattering: 1.8%; Fe56 inelastic scattering: 0.9% (*neither U238 fission nor U235 fission*).
ERALIB1: Various isotopes and reactions.

Most important contributions to the data uncertainty of F49/F25:
JEFF-3.1/BOLNA:U238 inelastic scattering: 0.5%; U235 fission: 0.5%; Pu239 fission: 0.4%.
JEF-2.2: Pu239 fission: 2.3%.
ERALIB1: Pu239 fission: 0.3%.

Most important contributions to the data uncertainty of C28/F25:
JEFF-3.1/BOLNA: U238 capture: 1.9%.
JEF-2.2: U238 capture: 1.1%; U235 fission: 1.0%.
ERALIB1: U238 capture: 0.3%; U235 fission: 0.2%.

ZPPR-9 (continued)

ZPPR-9/ Library	Calculated parameter	Corrected calculated parameter	1σ-uncertainty (%)	Experiment /1σ-uncertainty (%)
Na void (Step 3)				
JEFF-3.1/BOLNA	28.01	28.43	**67.60**	29.39 cents/1.225
JEF-2.2	30.15	30.60	**74.06**	
ERALIB1	26.21	26.61	7.51	
Na void (Step 5)				
JEFF-3.1/BOLNA	36.88	27.51	**91.40**	31.68 cents/1.136
JEF-2.2	40.62	30.30	**97.45**	
ERALIB1	35.22	26.28	9.97	
β_{eff}				
JEFF-3.1	0.003812	Given β_{eff}: 0.00355		
JEF-2.2	0.003816			

Similar uncertainties for JEFF-3.1/BOLNA and JEF-2-2.
However: Compensating effects between *U238 inelastic scattering* and *Pu239 fission*.

ZPPR-9 (continued)

Most important contributions to the data uncertainty of Na void Step 3 (JEFF-3.1/BOLNA):

Reaction/ Isotope	Capture	Elastic scattering	Inelastic scattering	Fission	ν	Total
Relative 1σ–uncertainty,% (> 1%, ν: > 0.1%)						
U235	1.3				0.5	1.4
U238	**28.2**		**54.3**	2.4	**8.3**	**61.6**
Pu239	**13.9**		3.1	**11.5**	**6.7**	**19.5**
Pu240	2.8			2.6	**3.2**	5.0
Pu241				4.7	0.2	4.7
Ni58	1.6					1.8
Fe56	3.3		7.5			8.3
Na23		2.3	5.4			5.9
O16	**11.7**	9.9	1.7			**15.3**

ZPPR-9 (continued)

Most important contributions to the data uncertainty of Na void Step 3 (JEF-2.2):

Reaction/ Isotope	Capture	Elastic scattering	Inelastic scattering	Fission	ν	Total
Relative 1σ–uncertainty,% (> 1%, ν: > 0.1%)						
U235				2.0	0.2	2.0
U238	**13.5**		**15.7**	9.3	**10.0**	**24.8**
Pu239	**12.3**		1.6	**61.0**	**24.7**	**67.0**
Pu240	3.2			5.0	**1.7**	6.2
Pu241				2.3	0.4	2.4
Cr52			1.7			2.0
Ni58	1.2					1.5
Fe56	2.4	2.3	6.5			7.3
Na23		5.1	**13.5**			**14.5**
O16	4.4	6.6				8.0

ZPPR-9 (continued)

Most important contributions to the data uncertainty of Na void Step 5 (JEFF-3.1/BOLNA):

Reaction/ Isotope	Capture	Elastic scattering	Inelastic scattering	Fission	ν	Total
Relative 1σ–uncertainty,% (> 1%, ν: > 0.1%)						
U235	1.7				0.6	1.9
U238	**37.7**		**73.8**	3.2	**10.9**	**83.4**
Pu239	**18.7**		4.2	**15.5**	**9.0**	**26.2**
Pu240	3.7			3.5	**4.2**	6.6
Pu241				6.3	0.3	6.3
Ni58	2.2					2.4
Fe56	4.4	1.2	**10.2**			**11.2**
Na23		3.2	7.5			8.3
O16	**15.5**	**13.4**	2.3			**20.6**

ZPPR-9 (continued)

Most important contributions to the data uncertainty of Na void Step 5 (JEF-2.2):

Reaction/ Isotope	Capture	Elastic scattering	Inelastic scattering	Fission	ν	Total
Relative 1σ–uncertainty,% (> 1%, ν: > 0.1%)						
U235				2.6	0.3	2.7
U238	**17.7**		**20.8**	**12.0**	**12.9**	**32.5**
Pu239	**16.3**		2.2	**80.2**	**32.5**	**88.1**
Pu240	4.2			6.5	**2.3**	8.1
Pu241				3.0	0.5	3.1
Cr52		1.3	2.2			2.7
Ni58	1.5		1.1			1.9
Fe56	3.2	3.2	8.6			9.3
Na23		7.0	**18.2**			**19.5**
O16	5.8	8.9				**10.7**

JOYO

JOYO/ Library	Calculated parameter	Corrected calculated parameter	1σ-uncertainty (%)	Experiment /1σ-uncertainty (%)
k_{eff}				
JEFF-3.1/BOLNA	1.00306	1.00413	1.253	1.00105/0.18
JEF-2.2	1.00169	1.00276	0.982	
ERALIB1	1.00000	1.00107	0.156	

Most important contributions to the data uncertainty of k_{eff}:

JEFF-3.1/BOLNA: U235 capture: 1.1%.

JEF-2.2: *Pu239 fission*: 0.7%.

ERALIB1: Pu239 fission: 0.1%.

ABR core

ABR startup oxide core Library	k_{eff}	1σ-uncertainty (%)
JEFF-3.1/BOLNA	1.01450	1.017
JEF-2.2	1.00657	1.661
ERALIB-1	1.01436	0.192
ABR recycled oxide core Library	k_{eff}	1σ-uncertainty (%)
JEFF-3.1/BOLNA	1.00574	1.489
JEF-2.2	0.99078	1.539
ERALIB-1	0.99981	0.384
ABR startup metal core Library	k_{eff}	1σ-uncertainty (%)
JEFF-3.1/BOLNA	1.00054	1.092
JEF-2.2	0.99717	1.817
ERALIB-1	1.00292	0.284

ABR core (continued)

Most important contributions to the data uncertainty of k_{eff} (oxide core):
JEFF-3.1/BOLNA: *U238 inelastic scattering*: 0.7%.
JEF-2.2: *Pu239 fission*: 1.4%.
ERALIB1: Pu239 fission: 0.1%.

Most important contributions to the data uncertainty of k_{eff} (oxide core, recycled):
JEFF-3.1/BOLNA: *U238 inelastic scattering*: 0.8%.
JEF-2.2: *Pu239 fission*: 1.0%.
ERALIB1: Pu238 fission: 0.2%.
(The remaining parts are coming from a variety of reactions and nuclides, the MA being important in each case).

Most important contributions to the data uncertainty of k_{eff} (metal core):
JEFF-3.1/BOLNA: *U238 inelastic scattering*: 0.9%.
JEF-2.2: *Pu239 fission*: 1.6%.
ERALIB1: Pu239 fission: 0.2%.

FBR core (RZ simplified model)

FBR core/ Library	Calculated parameter	Quoted value	1σ-uncertainty (%)
k_{eff}			
JEFF-3.1/BOLNA	1.05838	1.0522	1.618
JEF-2.2	1.04856		1.471
ERALIB1	1.05812		0.187
Na void reactivity ($)			
JEFF-3.1/BOLNA	3.89	4.3	8.62
JEF-2.2	4.12		7.06
ERALIB1	3.63		3.71
Doppler constant			
JEFF-3.1/BOLNA	-0.0102	-0.01	5.18
JEF-2.2	-0.0096		4.97
ERALIB1	-0.0093		2.24
β_{eff}			
JEFF-3.1	0.003943		
JEF-2.2	0.003914		

FBR core (continued)

Most important contributions to the data uncertainty of k_{eff}:
JEFF-3.1/BOLNA: *U238 inelastic scattering*: 0.9%; U238 capture: 0.4%.
JEF-2.2: *Pu239 fission*: 1.0%.
ERALIB1: Pu239 fission: 0.1%.

Most important contributions to the data uncertainty of the void reactivity,
JEFF-3.1/BOLNA:

Reaction/Isotope	Capture	Elastic scattering	Inelastic scattering	Fission	ν	Total
Relative 1σ–uncertainty,% (> 1%, ν: > 0.1%)						
U238	2.6		**4.6**		0.3	**5.2**
Pu239	1.5			1.7	0.4	2.3
Pu240					0.5	1.0
Pu241				**5.7**	0.1	**5.8**
Fe56	1.3					1.5
Na23		7.0	1.4			1.5
O16		1.3				1.6

FBR core (continued)

Most important contributions to the data uncertainty of the Doppler constant, JEFF-3.1/BOLNA:

Reaction/Isotope	Capture	Elastic scattering	Inelastic scattering	Fission	ν	Total
Relative 1σ–uncertainty,% (> 1%, ν: > 0.1%)						
U238	1.6		**3.1**		0.3	**3.5**
Pu239					0.2	0.9
Pu240					0.4	0.6
Pu241				**3.0**		**3.0**
O16		1.5				1.5

Conclusions

JEFF-3.1/BOLNA in general leads to satisfactory predictions of experimental values in the sense that there is a common domain for the calculational and experimental ranges by consistently considering 1σ standard deviations.

However, this overlap often results from the fact that data uncertainties are much larger than experimental uncertainties.
In addition, and as a consequence, calculational uncertainties do not match target uncertainties.

There is anyways a significant improvement as compared to the use of JEF-2.2.

The use of ERALIB-1 (adjusted JEF-2.2 data) significantly reduces the nuclear data uncertainty, but the computed values more frequently lie outside the experimental range. Moreover, the correlation matrices were found not positive definite, clearly resulting in underestimations of these uncertainties.

These findings certainly support the proposed adjustment exercise.