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Fission Spectrum Related Uncertainties

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Abstract: The paper presents a preliminary uncertainty analysis related to potential uncertainties on the fission spectrum data. Consistent results are shown for a reference fast reactor design configuration and for experimental thermal configurations. However the results obtained indicate the need for further analysis, in particular in terms of fission spectrum uncertainty data assessment.

Introduction

Sensitivity coefficients for the multiplication factor associated to the fission spectrum are calculated according to the formula:

$$S_{k_{eff}(\chi),i,g,d} = \left. \frac{\int_d \chi^*_{i,g,d} \Phi^*_{g,d} \times \left[\nu_{i,g',d} \Sigma_{f_{i,g',d}} \Phi_{g',d} \right] dr}{\int \sum_i \left[\chi_{i,g'} \Phi^*_{g'} \right] \times \left[\nu_{i,g'} \Sigma_{f_{i,g'}} \Phi_{g'} \right] dr} \right|_{\substack{i=\text{isotope} \\ g,g'=\text{energy group} \\ d=\text{domain}}} , \qquad (1)$$

where $\chi^*_{i,g,d} = \chi_{i,g,d} \frac{\langle \nu \Sigma_{f_{i,d}} \Phi_d \rangle}{\langle \nu \Sigma_{f_d} \Phi_d \rangle}$, $[\ ]$ denotes the integration over the energy (summation over the groups g'), while $\langle\ \rangle$ denotes the integration over energy and space. After computing the sensitivity coefficients, the fission spectrum related uncertainties are successively determined using the classical formula $\Delta R_0^2 = S^+_{k_{eff}(\chi)} D S_{k_{eff}(\chi)}$, where D is the dispersion matrix containing the covariance data.

Sensitivity coefficient results

The following sensitivity coefficients have been calculated for the ABTR [1] multiplication factor with the ERANOS code system [2]. Table 1 gives the breakdown by energy group for Pu-239 and the total values by isotope. The sensitivity coefficients shown in the tables are the total over the reactor. It can be observed that, as expected, the total isotope sensitivity for the fission spectrum has the same value of ν; the distribution by energy group is however different for each isotope (see case of Pu-239). Additionally, the overall k_{eff} sensitivity to the fission spectrum (and to ν) is practically 100% (Table 1 gives $\Delta k/k^2$ sensitivities and for the ABTR under study k_{eff} = 1.034472).

Table 1. *Δk/k²: Sensitivity Coefficients for ABTR*

		Pu-239: Breakdown by Energy Group						
Gr.	**Energy** [(a)]	σ_{capt}	σ_{el}	ν	σ_{inel}	σ_{fiss}	χ	**Total**
1	**19.6 MeV**	0.00	0.00	0.45	-0.01	0.30	3.24	3.98
2	**6.07 MeV**	-0.01	0.01	4.51	-0.13	3.03	29.49	36.90
3	**2.23 MeV**	-0.03	0.02	4.62	-0.08	3.08	18.80	26.41
4	**1.35 MeV**	-0.21	0.09	15.02	-0.05	10.42	20.08	45.36
5	**498 keV**	-0.58	0.17	20.32	-0.01	14.31	6.01	40.22
6	**183 keV**	-0.74	0.13	16.15	-0.02	11.68	1.37	28.57
7	**67.4 keV**	-0.55	0.03	8.00	-0.01	5.99	0.28	13.75
8	**24.8 keV**	-0.59	0.02	5.32	0.01	4.04	0.06	8.87
9	**9.12 keV**	-0.34	0.00	1.67	0.00	1.24	0.02	2.58
10	**2.03 keV**	-0.51	0.00	2.19	0.00	1.56	0.00	3.24
11	**454 eV**	-0.21	0.00	0.79	0.00	0.49	0.00	1.06
12	**22.6 eV**	-0.03	0.00	0.11	0.00	0.06	0.00	0.14
13	**4 eV**	0.00	0.00	0.04	0.00	0.03	0.00	0.07
14	**0.54 eV**	0.00	0.00	0.01	0.00	0.00	0.00	0.01
15	**0.1 eV**	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total		-3.80	0.47	79.20	-0.29	56.24	79.35	211.17

(a) Upper energy boundary

	Total Sensitivity - Breakdown by Isotope							
Isotope	σ_{capt}	σ_{el}	ν	σ_{inel}	σ_{fiss}	$\sigma_{n.2n}$	χ	**Total**
U235	-0.04	0.00	0.56	-0.01	0.37	0.00	0.56	1.44
U238	-13.84	2.72	12.22	-4.20	7.42	0.08	12.08	16.50
Pu238	-0.01	0.00	0.16	0.00	0.11	0.00	0.16	0.42
Pu239	-3.80	0.47	79.20	-0.29	56.24	0.00	79.35	211.17
Pu240	-0.62	0.07	2.65	-0.05	1.80	0.00	2.65	6.51
Pu241	-0.07	0.01	1.51	0.00	1.09	0.00	1.51	4.04
Pu242	-0.03	0.00	0.10	0.00	0.07	0.00	0.10	0.24
Np237	-0.08	0.00	0.10	0.00	0.07	0.00	0.10	0.18
Am241	-0.12	0.00	0.11	0.00	0.08	0.00	0.10	0.17
Am242m	0.00	0.00	0.02	0.00	0.02	0.00	0.02	0.07
Am243	-0.02	0.00	0.02	0.00	0.01	0.00	0.01	0.02
Cm242	0.00	0.00	0.01	0.00	0.01	0.00	0.01	0.02
Cm244	0.00	0.00	0.01	0.00	0.01	0.00	0.01	0.02
Cm245	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
Fe56	-1.38	5.18	0.00	-1.59	0.00	0.00	0.00	2.22
Cr52	-0.17	1.25	0.00	-0.17	0.00	0.07	0.00	0.98
Ni58	-0.05	0.12	0.00	-0.01	0.00	0.00	0.00	0.06
Zr90	-0.14	0.49	0.00	-0.21	0.00	0.00	0.00	0.14
Na23	-0.12	2.03	0.00	-0.42	0.00	0.00	0.00	1.49
B10	-0.52	0.01	0.00	0.00	0.00	0.00	0.00	-0.52
Total	-21.01	12.37	96.66	-6.96	67.29	0.16	96.66	245.18

Fission spectra covariance matrices

The information on the fission spectra covariance matrices is available in the DOSCOV package [3] and in the JENDL-3.2 and -3.3 [4,5] evaluations. In the DOSCOV package, dating back to ~1980, the covariance data for the U-235 fission spectrum were obtained assuming the standard deviations of 1.2% and 5.9% for the Watt spectrum parameters *a* and *b*, respectively, and the correlation of -0.21 between them. For the purpose of these studies the covariance matrices were converted from the DOSCOV 24-group structure to those needed using the ANGELO code [6].

More recently, the covariance matrices for several isotopes, including U-235, U-238, Pu-239, were prepared in the JENDL-3.2 and -3.3 [2,3] evaluations. The data were processed using the ERROR-J 2.3 code [7].

The JENDL3.3 fission spectrum covariance matrix for Pu-239 is presented in Table 2 in a 15 energy group structure.

Table 2. *Pu-239 JENDL3.3 Variance/Covariance Data (ABTR)*

			Covariances														
		Group	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
Variances (%)	**Gr.**	**Energy** [(a)]	**19.6 MeV**	**6.07 MeV**	**2.23 MeV**	**1.35 MeV**	**498 keV**	**183 keV**	**67.4 keV**	**24.8 keV**	**9.12 keV**	**2.03 keV**	**454 eV**	**22.6 eV**	**4 eV**	**0.54 eV**	**0.1 eV**
9.58	**1**	**19.6 MeV**	1.000	0.787	-0.323	-0.905	-0.665	-0.608	-0.592	-0.589	-0.589	-0.590	-0.594	-0.595	-0.595	-0.596	-0.596
7.12	**2**	**6.07 MeV**	0.787	1.000	0.329	-0.975	-0.984	-0.968	-0.963	-0.962	-0.962	-0.963	-0.964	-0.964	-0.964	-0.964	-0.964
1.03	**3**	**2.23 MeV**	-0.323	0.329	1.000	-0.110	-0.491	-0.554	-0.571	-0.574	-0.574	-0.574	-0.569	-0.568	-0.568	-0.568	-0.568
5.03	**4**	**1.35 MeV**	-0.905	-0.975	-0.110	1.000	0.919	0.888	0.879	0.877	0.877	0.877	0.880	0.880	0.881	0.881	0.881
6.62	**5**	**498 keV**	-0.665	-0.984	-0.491	0.919	1.000	0.997	0.996	0.995	0.995	0.995	0.996	0.996	0.996	0.996	0.996
8.92	**6**	**183 keV**	-0.608	-0.968	-0.554	0.888	0.997	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
8.21	**7**	**67.4 keV**	-0.592	-0.963	-0.571	0.879	0.996	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
7.30	**8**	**24.8 keV**	-0.589	-0.962	-0.574	0.877	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
12.59	**9**	**9.12 keV**	-0.589	-0.962	-0.574	0.877	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
12.16	**10**	**2.03 keV**	-0.590	-0.963	-0.574	0.877	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
25.09	**11**	**454 eV**	-0.594	-0.964	-0.569	0.880	0.996	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.61	**12**	**22.6 eV**	-0.595	-0.964	-0.568	0.880	0.996	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.05	**13**	**4 eV**	-0.595	-0.964	-0.568	0.881	0.996	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.00	**14**	**0.54 eV**	-0.596	-0.964	-0.568	0.881	0.996	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.00	**15**	**0.1 eV**	-0.596	-0.964	-0.568	0.881	0.996	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

(a) Upper energy boundary

The DOSCOV fission spectrum covariance matrix is presented in Table 3 for U-235 in a 15 energy group structure. In the present study, as demonstrative example, the same matrix has been used for Pu-239.

Table 3. *U-235 DOSCOV Variance/Covariance Data (ABTR)*

			Covariances														
		Group	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
Variances (%)	**Gr.**	**Energy [(a)]**	**19.6 MeV**	**6.07 MeV**	**2.23 MeV**	**1.35 MeV**	**498 keV**	**183 keV**	**67.4 keV**	**24.8 keV**	**9.12 keV**	**2.03 keV**	**454 eV**	**22.6 eV**	**4 eV**	**0.54 eV**	**0.1 eV**
11.33	**1**	**19.6 MeV**	1.000	1.002	-0.674	-1.011	-1.002	-0.991	-0.991	-0.991	-0.991	-0.991	-0.991	-0.991	-0.991	-0.991	-0.991
2.85	**2**	**6.07 MeV**	0.969	1.000	-0.590	-1.012	-1.003	-0.991	-0.991	-0.991	-0.991	-0.991	-0.991	-0.991	-0.991	-0.991	-0.991
0.31	**3**	**2.23 MeV**	-0.770	-0.620	1.000	0.649	0.616	0.618	0.614	0.613	0.612	0.612	0.612	0.612	0.612	0.612	0.612
1.93	**4**	**1.35 MeV**	-0.992	-1.000	0.596	1.000	1.002	1.010	1.010	1.010	1.010	1.010	1.010	1.010	1.010	1.010	1.010
2.98	**5**	**498 keV**	-0.974	-0.999	0.564	0.998	1.000	1.009	1.009	1.009	1.009	1.009	1.009	1.009	1.009	1.009	1.009
3.46	**6**	**183 keV**	-0.952	-0.990	0.559	0.990	0.991	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.64	**7**	**67.4 keV**	-0.950	-0.990	0.559	0.990	0.991	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.71	**8**	**24.8 keV**	-0.950	-0.990	0.559	0.990	0.991	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.73	**9**	**9.12 keV**	-0.949	-0.990	0.559	0.990	0.991	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.74	**10**	**2.03 keV**	-0.949	-0.990	0.559	0.990	0.991	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.74	**11**	**454 eV**	-0.949	-0.990	0.559	0.990	0.991	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.74	**12**	**22.6 eV**	-0.949	-0.990	0.559	0.990	0.991	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.74	**13**	**4 eV**	-0.949	-0.990	0.559	0.990	0.991	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.74	**14**	**0.54 eV**	-0.949	-0.990	0.559	0.990	0.991	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.74	**15**	**0.1 eV**	-0.949	-0.990	0.559	0.990	0.991	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

[(a)] Upper energy boundary

Uncertainty results

Table 4 shows the breakdown of the calculated uncertainty coefficients by energy group for Pu-239 and the total uncertainties by isotope. Results for the fission spectrum are obtained with the JENDL3.3 covariance data (only U-235 and Pu-239 matrices were available), while for other cross-sections the BOLNA dispersion matrix [8] is used. It is observed that the total uncertainty associated with the fission spectrum is dramatically important, an order of magnitude higher than the ν total contribution. Consequently, the overall uncertainty on the multiplication factor significantly increases (from 0.92% to 4.01%) becoming desperately out of the required accuracies (0.3%).

Table 4. *$\Delta k/k^2$: Uncertainty Coefficients (ABTR)*

		Pu-239: Breakdown by Energy Group						
Gr.	**Energy [(a)]**	σ_{capt}	σ_{el}	ν	σ_{inel}	σ_{fiss}	χ	**Total**
1	**19.6 MeV**	0.00	0.00	0.00	0.01	0.01	1.01	1.01
2	**6.07 MeV**	0.02	0.01	0.01	0.04	0.05	2.87	2.87
3	**2.23 MeV**	0.03	0.01	0.01	0.03	0.05	0.34	0.35
4	**1.35 MeV**	0.06	0.02	0.02	0.03	0.10	1.96	1.97
5	**498 keV**	0.11	0.02	0.05	0.01	0.13	1.21	1.22
6	**183 keV**	0.11	0.01	0.09	0.01	0.13	0.66	0.69
7	**67.4 keV**	0.09	0.00	0.06	0.01	0.08	0.29	0.32
8	**24.8 keV**	0.09	0.00	0.04	0.01i	0.06	0.13	0.17
9	**9.12 keV**	0.07	0.00	0.02	0.00	0.02	0.09	0.12
10	**2.03 keV**	0.01	0.00	0.00	0.00	0.02	0.03	0.04
11	**454 eV**	0.00	0.00	0.00	0.00	0.01	0.01	0.02
12	**22.6 eV**	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	**4 eV**	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	**0.54 eV**	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	**0.1 eV**	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total		0.23	0.03	0.13	0.06	0.24	3.90	3.92

	Total Uncertainty - Breakdown by Isotope							
Isotope	σ_{capt}	σ_{el}	ν	σ_{inel}	σ_{fiss}	$\sigma_{n.2n}$	χ	**Total**
U235	0.01	0.00	0.00	0.00	0.00	0.00	0.02	0.02
U238	0.26	0.20	0.14	0.69	0.04	0.00	0.00	0.77
Pu238	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.02
Pu239	0.23	0.03	0.13	0.06	0.24	0.00	3.90	3.92
Pu240	0.06	0.00	0.08	0.01	0.09	0.00	0.00	0.13
Pu241	0.01	0.00	0.00	0.00	0.12	0.00	0.00	0.12
Pu242	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.01
Np237	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
Am241	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.01
Fe56	0.07	0.08	0.00	0.24	0.00	0.00	0.00	0.27
Cr52	0.01	0.06	0.00	0.00	0.00	0.01	0.00	0.06
Zr90	0.01	0.01	0.00	0.03	0.00	0.00	0.00	0.04
Na23	0.02	0.05	0.00	0.07	0.00	0.00	0.00	0.08
B10	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.04
Total	0.36	0.23	0.20	0.73	0.29	0.01	3.90	4.01

[(a)] Upper energy boundary

Table 5 shows the results with the DOSCOV covariance matrix for the fission spectrum (only U-235 and Pu-239 matrices were available). The fission spectrum related uncertainties are lower than in the previous case but still very high.

Table 5. *$\Delta k/k^2$: Uncertainty Coefficients (ABTR)*

Gr.	Energy [(a)]	Pu-239: Breakdown by Energy Group						
		σ_{capt}	σ_{el}	ν	σ_{inel}	σ_{fiss}	χ	Total
1	19.6 MeV	0.00	0.00	0.00	0.01	0.01	0.83	0.83
2	6.07 MeV	0.02	0.01	0.01	0.04	0.05	1.26	1.26
3	2.23 MeV	0.03	0.01	0.01	0.03	0.05	0.26	0.27
4	1.35 MeV	0.06	0.02	0.02	0.03	0.10	0.86	0.86
5	498 keV	0.11	0.02	0.05	0.01	0.13	0.58	0.60
6	183 keV	0.11	0.01	0.09	0.01	0.13	0.30	0.36
7	67.4 keV	0.09	0.00	0.06	0.01	0.08	0.14	0.19
8	24.8 keV	0.09	0.00	0.04	0.01i	0.06	0.07	0.13
9	9.12 keV	0.07	0.00	0.02	0.00	0.02	0.03	0.08
10	2.03 keV	0.01	0.00	0.00	0.00	0.02	0.01	0.02
11	454 eV	0.00	0.00	0.00	0.00	0.01	0.00	0.01
12	22.6 eV	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	4 eV	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	0.54 eV	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	0.1 eV	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total		0.23	0.03	0.13	0.06	0.24	1.87	1.91

Isotope	Total Uncertainty - Breakdown by Isotope							
	σ_{capt}	σ_{el}	ν	σ_{inel}	σ_{fiss}	$\sigma_{n.2n}$	χ	Total
U235	0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.02
U238	0.26	0.20	0.14	0.69	0.04	0.00	0.00	0.77
Pu238	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.02
Pu239	0.23	0.03	0.13	0.06	0.24	0.00	1.87	1.91
Pu240	0.06	0.00	0.08	0.01	0.09	0.00	0.00	0.13
Pu241	0.01	0.00	0.00	0.00	0.12	0.00	0.00	0.12
Pu242	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.01
Np237	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
Am241	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.01
Fe56	0.07	0.08	0.00	0.24	0.00	0.00	0.00	0.27
Cr52	0.01	0.06	0.00	0.00	0.00	0.01	0.00	0.06
Zr90	0.01	0.01	0.00	0.03	0.00	0.00	0.00	0.04
Na23	0.02	0.05	0.00	0.07	0.00	0.00	0.00	0.08
B10	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.04
Total	0.36	0.23	0.20	0.73	0.29	0.01	1.87	2.09

[(a)] Upper energy boundary

KRITZ critical light water benchmark analysis

Cross-section sensitivity and uncertainty analyses of several KRITZ UO_2 and MOX critical configurations [9] were performed in the scope of the OECD international benchmark exercise. These studies, based on the SUSD3D [10] cross-section sensitivity and uncertainty package, addressed among other sources of uncertainty also those linked to the fission spectra [11]. The calculated uncertainties in k_{eff} due to the uncertainties in the fission spectra of U-235, U-238 and Pu-239 are presented in Table 6.

It can be observed that the uncertainties vary only slightly between different KRITZ configurations. Subsequently it seems that the discrepancy between the calculated and measured k_{eff}, largely varying with the configuration and the temperature, cannot be explained by the fission spectra uncertainties. Furthermore, compared to the observed discrepancies between the calculations and experiments, of the order of ~0.5 %, these uncertainties seem largely overestimated, indicating either some error compensation effects, or too-conservative covariance matrix estimations.

Table 6. *Fission Spectra Related Uncertainties for the KRITZ benchmarks.*

	Impact of fission spectra uncertainty [%]				
	KRITZ-2.1c	KRITZ-2.1h	KRITZ-2.13c	KRITZ-2.13h	KRITZ-2.19c
U235 (DOSCOV)	1.59	1.58	1.62	1.61	0.09
U235 (JENDL3.3)	4.06	4.03	4.14	4.11	0.24
U238 (JENDL3.3)	0.61	0.71	0.48	0.53	0.19
Pu239 (JENDL3.3)	-	-	-	-	3.68
Total (JENDL3.3)	4.10	4.09	4.16	4.14	3.70

Conclusions

The impact of the uncertainties in the fission spectra was evaluated for an actinide burner Na-cooled fast reactor (ABTR) as well as for several KRITZ critical benchmark configurations. The information on the fission spectra covariance matrices was taken from the JENDL-3.3 [4,5] evaluation and the DOSCOV package [3]. Large differences were observed between the two with the uncertainties in k_{eff} as high as 1.5 – 4 %. The results show rather small differences between different reactor systems (fast, light water) and different configurations (UO_2, MOX). Furthermore, compared to the observed discrepancies between the calculations and experiments for KRITZ, of the order of ~0.5 %, these uncertainties seem largely overestimated, indicating either some error compensation effects (due to cross-section adjustments involving nu-bar, absorption etc.), or too-conservative covariance matrix estimations.

Possible inconsistencies in correlation matrix were observed.

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