

*6th Meeting of WPEC Subgroup 33 on
Methods and issues for the combined use of integral experiments and covariance data*

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Comparison of Adjustment Results Using Covariances of JENDL-4.0 and COMMARA 2.0

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Outline of Adjustment by JAEA

- ✓ Base library: **JENDL-4.0** released in May 2010,
- ✓ Energy structure: 33 group structure of SG33 standard,
- ✓ Isotopes to be adjusted: B-10, O-16, Na-23, Fe-56, Cr-52, Ni-58, U-235, -238, Pu-239, -240, -241 (Total 11),
- ✓ Reactions to be adjusted: Elastic, Total inelastic, Capture (n, alpha for B-10), Fission, Nu-total, **Chi-p**, **Mu**, **Nu-d** (Total 8),
- ✓ Nuclear data covariance: **JENDL-4.0** processed with NJOY,
- ✓ Integral data for adjustment: JEZEBEL-Pu239 (keff, F28/F25, F49/F25, F37/F25), -Pu240 (keff), FLATTOP-Pu (keff, F28/F25, F37/F25), ZPR-6/7 (keff, F28/F25, F49/F25, C28/F25), -High Pu240 (keff), ZPPR-9 (keff, F28/F25, F49/F25, C28/F25, Na void reactivity (Step 3, 5)), JOYO Mk-I (keff) (Total 20).



Analytical Method applied to obtain C/E values

No.	Core	Parameter	Case J (As-built MC for ZPPR-9)
1, 2, 3, 4	JEZEBEL-Pu	keff, F28/F25, F49/F25, F37/F25	ICSBEP benchmark model calculation with continuous energy Monte Carlo (MC) code, MVP
5	" -Pu240	keff	
6, 7, 8	FLATTOP-Pu	keff, F28/F25, F37/F25	
9, 10, 11, 12	ZPR-6/7	keff, F28/F25, F49/F25, C28/F25	2D MC of simple model + Corrective factor (C.F.) by INL
13	" -High Pu240	keff	
14	ZPPR-9	keff	As-Built MC by JAEA
15, 16, 17		F28/F25, F49/F25, C28/F25	2D MC + C.F. by INL
18, 19		Na void reactivity (Step 3, 5)	As-Built MC by JAEA
20	JOYO Mk-I	keff	2D MC + C.F. by JAEA (C.F. by INL=0.99666, by JAEA=0.99515)



Integral Data for Adjustment

(Case J: As-built Monte Carlo results for ZPPR-9 by JAEA)

Case J) Adjustment Data with As-built Monte Carlo Results for ZPPR-9 by JAEA										
No.	Core	Parameter	Parameter value		C/E value	Relative uncertainty (%)			2D Monte Carlo by JAEA	Corrective factor by INL
			Experiment	Calculation		Experiment	Analytical modeling	Sum		
1	JEZEBEL-Pu239	keff	1.00000	0.99865	0.9987	0.200	0.027	0.202		
2		F28/F25	0.2133	0.20660	0.9686	1.1	0.94	1.447		
3		F49/F25	1.4609	1.43701	0.9836	0.9	0.75	1.172		
4		F37/F25	0.9835	0.96322	0.9794	1.4	0.80	1.612		
5	JEZEBEL-Pu240	keff	1.00000	0.99839	0.9984	0.200	0.027	0.202		
6	FLATTOP-Pu	keff	1.00000	0.99859	0.9986	0.300	0.033	0.302		
7		F28/F25	0.1799	0.17582	0.9773	1.1	0.84	1.384		
8		F37/F25	0.8561	0.84968	0.9925	1.4	0.69	1.561		
9	ZPR-6/7	keff	1.00051	1.00579	1.0053	0.230	0.025	0.231	0.99158	1.01433
10		F28/F25	0.0223	0.0230	1.0336	3.0	2.24	3.74	0.02202	1.04673
11		F49/F25	0.9435	0.9237	0.9790	2.1	1.43	2.54	0.9359	0.9870
12		G28/F25	0.1323	0.1345	1.0167	2.4	1.22	2.69	0.1398	0.9625
13	ZPR-6/7 High-Pu240	keff	1.00080	1.00413	1.0033	0.220	0.030	0.222	0.98980	1.01448
14	ZPPR-9	keff	1.00080	1.00295	1.0021	0.117	0.020	0.119		
15		F28/F25	0.0207	0.02034	0.9828	2.7	2.09	3.41	0.02004	1.0152
16		F49/F25	0.9225	0.9217	0.9992	2.0	1.21	2.34	0.9261	0.9953
17		G28/F25	0.1296	0.1320	1.0188	1.9	1.39	2.35	0.1395	0.9465
18		Na void (Step 3)*	29.18	31.39	1.0759	1.9	5.26	5.59		
19		Na void (Step 5)*	31.30	33.34	1.0651	1.9	4.95	5.30		
20	JOYO Mk-I	keff	1.00105	0.99923	0.9982	0.180	0.028	0.182		

*Cent unit (beta value of ZPPR-9 by JENDL-4.0 = 0.003594)

***Note: Analytical modeling error is twice as the MC statistical error.**

- 1) **Black bold** – same with June 2010 meeting.
- 2) **Blue bold** – Specification change by INL or JAEA.
- 3) **Red bold** – 2D RZ Monte Carlo result by JAEA.
- 4) **Green bold** – (INL's MC²+JAEA's MC²)*1/2
- 5) **Pink bold** – As-built Monte Carlo result by JAEA.
- 6) **Brown bold** – Corrected by JAEA in October 2011.



Experimental Error Matrix V_e (Corrected in Oct. 2011)

No.	Core		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	
1	Jezebel - Pu239	keff	0.2																				
2		F28/F25	0	1.1																			
3		F49/F25	0	+0.23	0.9																		
4		F37/F25	0	+0.23	+0.32	1.4																	
5	Jezebel - Pu240	keff	0	0	0	0	0.2																
6	Flattop	keff	0	0	0	0	0	0.3															
7		F28/F25	0	0	0	0	0	0	1.1														
8		F37/F25	0	0	0	0	0	0	+0.23	1.4													
9	ZPR6-7	keff	0	0	0	0	0	0	0	0	0.23												
10		F28/F25	0	0	0	0	0	0	0	0	0	3.0											
11		F49/F25	0	0	0	0	0	0	0	0	0	+0.23	2.1										
12		C28/F25	0	0	0	0	0	0	0	0	0	+0.2	+0.32	2.4									
13	ZPR6-7 Pu240	keff	0	0	0	0	0	0	0	0	+0.13	0	0	0	0.22								
14	ZPPR-9	keff	0	0	0	0	0	0	0	0	+0.31	0	0	0	+0.30	0.117							
15		F28/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2.7						
16		F49/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+0.23	2.0					
17		C28/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+0.23	+0.32	1.9				
18		Na void (Step 3)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.9		
19	Na void (Step 5)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+0.41	1.9		
20	Joyo	keff	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.18

Symmetric

* Diagonal term: Error value (1 sigma, %)

** Non-diagonal term : Correlation factor (between -1 and +1)



Analytical Modeling Error Matrix V_m

No.	Core		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	
1	Jezebel - Pu239	keff	0.03																				
2		F28/F25	0	0.9																			
3		F49/F25	0	+0.5	0.8																		
4		F37/F25	0	+0.5	+0.5	0.8																	
5	Jezebel - Pu240	keff	0	0	0	0	0.03																
6	Flattop	keff	0	0	0	0	0	0.03															
7		F28/F25	0	0	0	0	0	0	0.8														
8		F37/F25	0	0	0	0	0	0	+0.5	0.7													
9	ZPR6-7	keff	0	0	0	0	0	0	0	0	0.03												
10		F28/F25	0	0	0	0	0	0	0	0	0	2.2											
11		F49/F25	0	0	0	0	0	0	0	0	0	+0.5	1.4										
12		C28/F25	0	0	0	0	0	0	0	0	0	+0.5	+0.5	1.2									
13	ZPR6-7 Pu240	keff	0	0	0	0	0	0	0	0	0	0	0	0	0.03								
14	ZPPR-9	keff	0	0	0	0	0	0	0	0	0	0	0	0	0	0.02							
15		F28/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2.1						
16		F49/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+0.5	1.2					
17		C28/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+0.5	+0.5	1.4				
18		Central Na void	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5.3		
19	Large Na void	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5.0		
20	Joyo	keff	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.03

Symmetric

* Diagonal term: Error value (1 sigma, %)

** Non-diagonal term : Correlation factor (between -1 and +1)



Results of Adjustment (Case J)

Result of Case J) Adjustment Data with As-built Monte Carlo Results for ZPPR-9 by JAEA

No.	Core	Parameter	C/E value		Relative uncertainty (%)		Nuclea-data-induced error (%)		Ratio of C/E-1 to prior total-error*
			Before	After	Experiment (Ve)	Analytical modeling (Vm)	Before (GMG)	After (GM'G)	
1	JEZEBEL-Pu239	keff	0.9987	0.9997	0.20	0.03	0.69	0.15	0.18
2		F28/F25	0.969	0.990	1.1	0.94	3.20	1.02	0.89
3		F49/F25	0.984	0.987	0.9	0.75	0.63	0.47	1.23
4		F37/F25	0.979	0.989	1.4	0.80	1.50	0.67	0.94
5	JEZEBEL-Pu240	keff	0.9984	1.0000	0.20	0.03	0.65	0.14	0.24
6	FLATTOP-Pu	keff	0.9986	1.0003	0.30	0.03	1.26	0.28	0.11
7		F28/F25	0.977	0.998	1.1	0.84	2.94	0.97	0.70
8		F37/F25	0.993	1.001	1.4	0.69	1.44	0.72	0.35
9	ZPR-6/7	keff	1.0053	1.0029 (1.0036)**	0.23	0.03	1.07	0.12 (0.16)**	0.48
10		F28/F25	1.034	1.027	3.0	2.24	4.95	1.91	0.54
11		F49/F25	0.979	0.976	2.1	1.43	1.21	0.84	0.75
12		C28/F25	1.017	1.009	2.4	1.22	3.61	1.24	0.37
13	ZPR-6/7 High-Pu240	keff	1.0033	1.0009 (1.0017)**	0.22	0.03	1.06	0.12 (0.15)**	0.30
14	ZPPR-9	keff	1.0021	1.0001 (1.0008)**	0.117	0.02	1.20	0.13 (0.15)**	0.17
15		F28/F25	0.983	0.974	2.7	2.09	5.45	2.10	0.27
16		F49/F25	0.999	0.996	2.0	1.21	1.24	0.85	0.03
17		C28/F25	1.019	1.011	1.9	1.39	3.72	1.26	0.43
18		Na void (Step 3)	1.076	1.034 (1.034)**	1.9	5.26	6.29	3.01 (2.99)**	0.90
19		Na void (Step 5)	1.065	1.013 (1.014)**	1.9	4.95	7.78	3.71 (3.67)**	0.69
20	JOYO Mk-I	keff	0.9982	0.9990	0.18	0.03	0.68	0.16	0.26

Chi-square/Freedom = 0.53

** Values in May 2011 Meeting.

* = (((C/E-1)**2)/(GMG+Ve+Vm)**1/2

1) Pink bold - Error value and/or correlation factors are corrected.

2) Brown bold - Corrected by JAEA in October 2011.

Parametric Survey of Covariances

0.53 Case J: Use of JENDL-4.0 covariances (Reference)

0.46 Case B0: Use of COMMARA 2.0 covariances , + J-4.0.

The missing covariance data are substituted by JENDL-4.0:

- Mu of U-235, U-238, Pu-239, Pu-240, Pu-241,
B-10, O-16, Cr-52, Ni-58.

(Mu of Na-23, Fe-56 are from COMMARA 2.0)

- Nu-d of U-235, U-238, Pu-239, Pu-240, Pu-241
(No Nu-d covariances in COMMARA 2.0)

0.47 Case B2: Use of COMMARA 2.0 covariances, only.

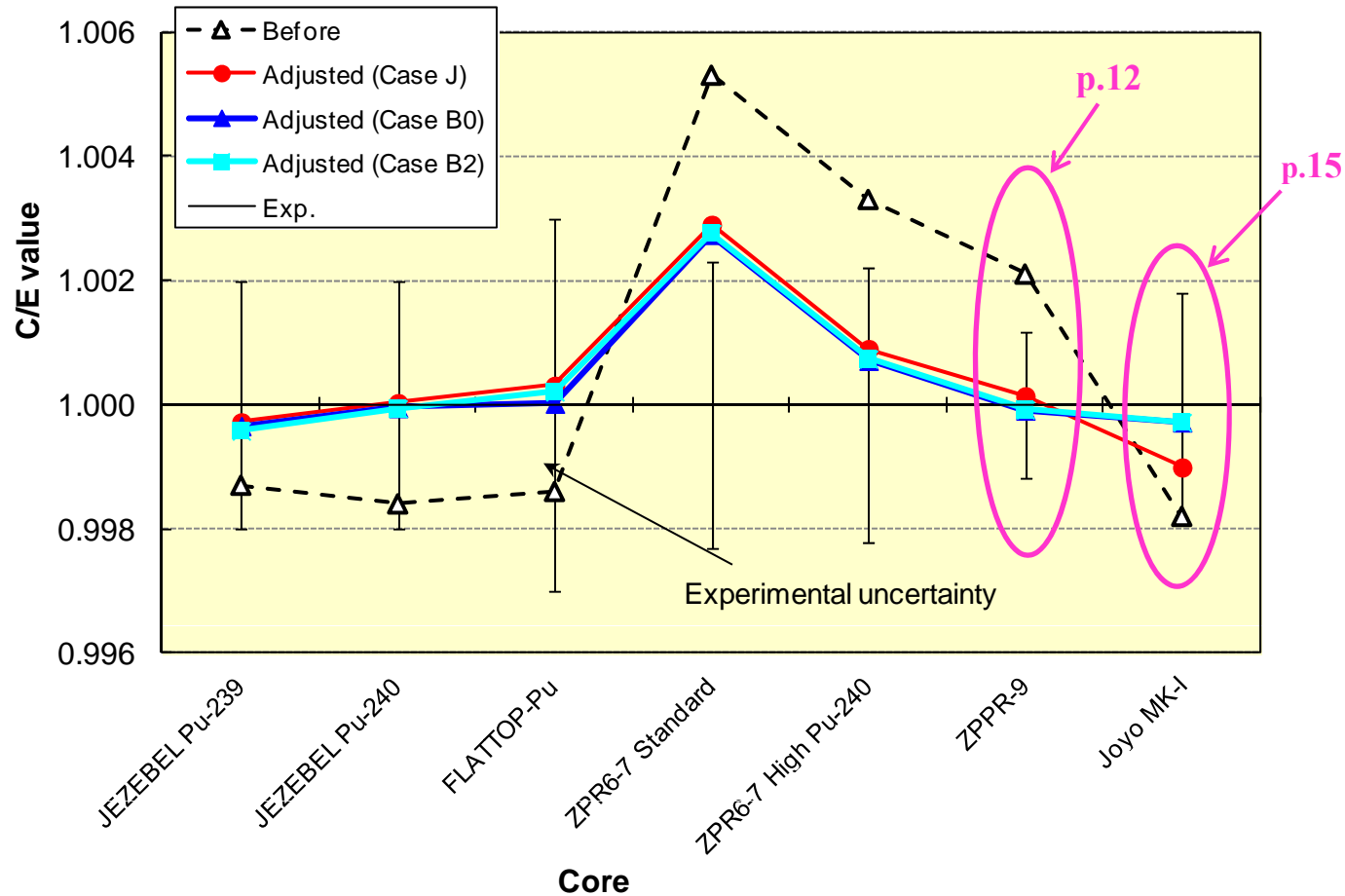


No JENDL-4.0 data.

(chi-square / number of freedom)



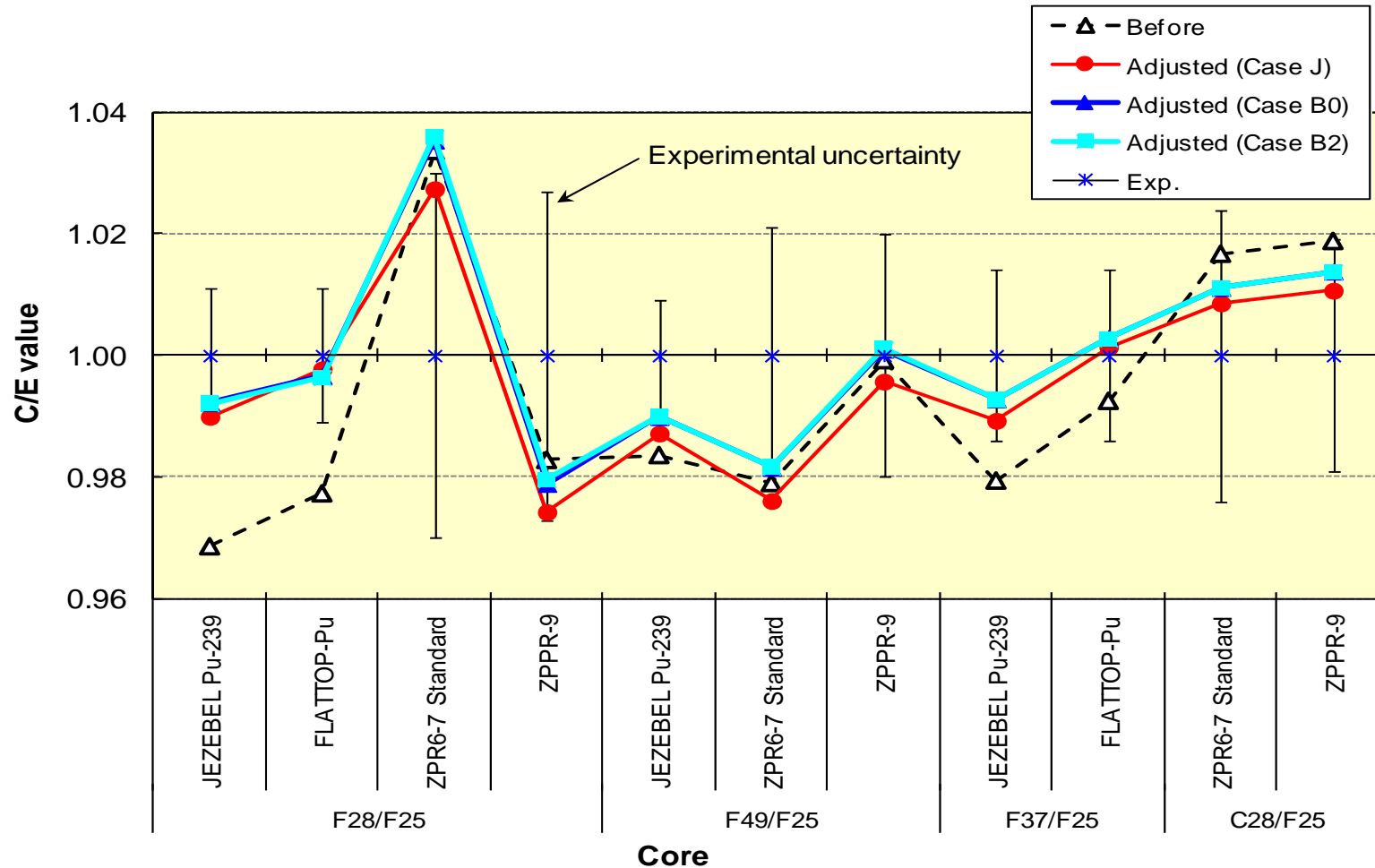
Change of C/E values (keff)



=> Three cases are almost identical for adjusted keff from small through large cores, except JOYO.



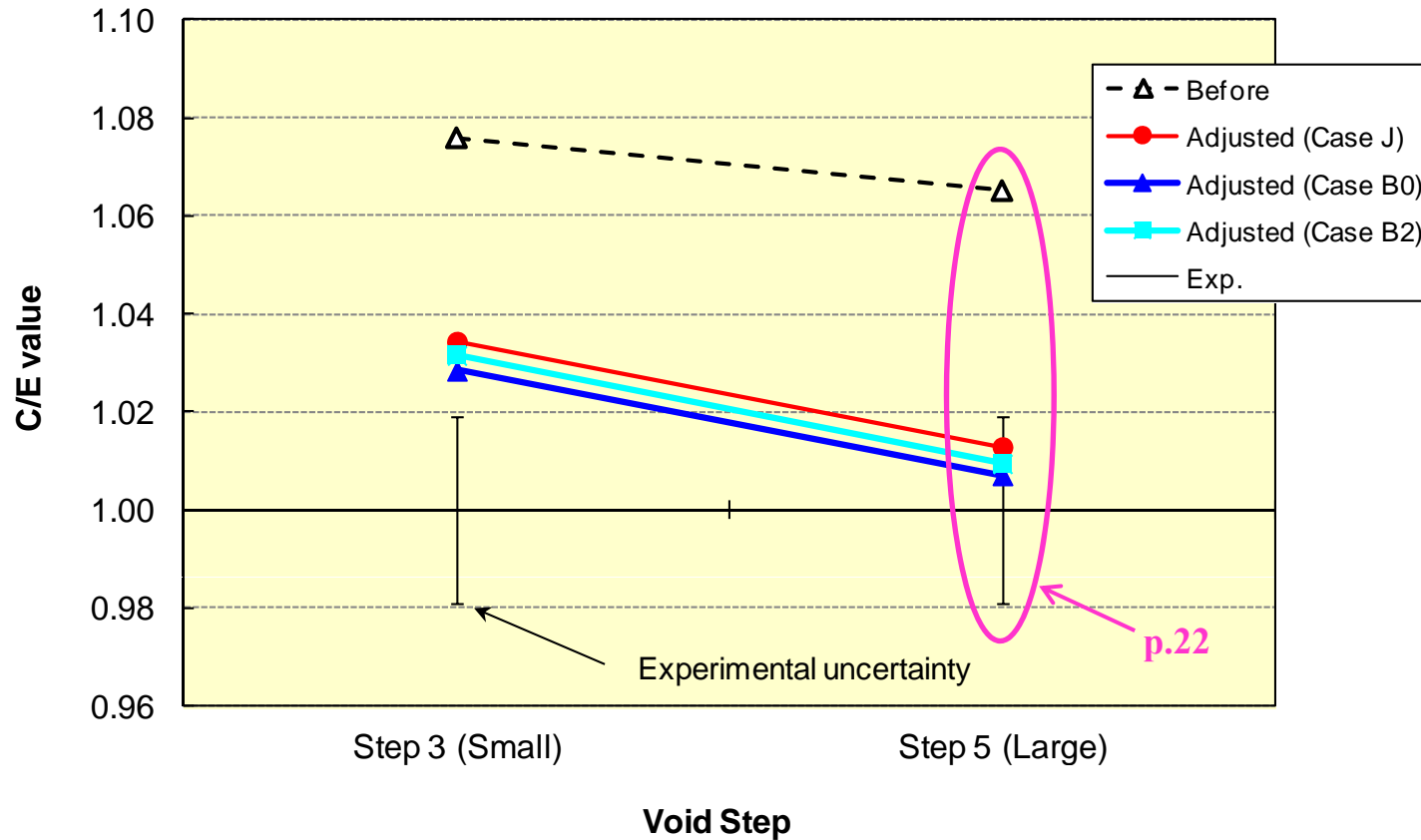
Change of C/E values (Reaction rate ratio)



⇒ **Three cases are similar, but a little bias between JENDL and COMMARA for every R.R. ratio, which is not affected by the prior C/E values.**



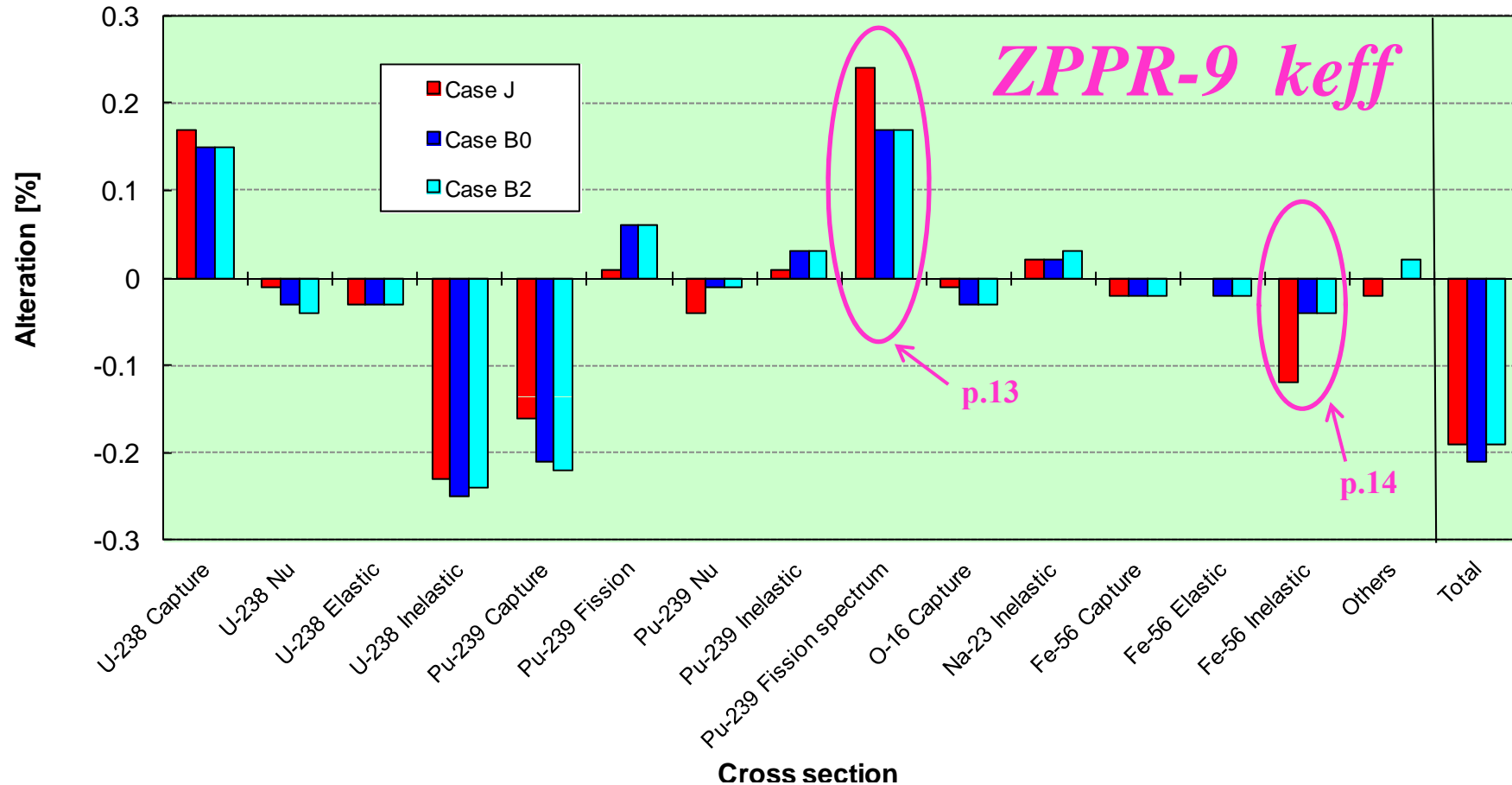
Change of C/E values (Na void reactivity)



⇒ **Case B0 seems a little better, and the slight effect of Nu-d adjustment can be observed.**

Contribution to C/E change (1)

ZPPR-9 keff

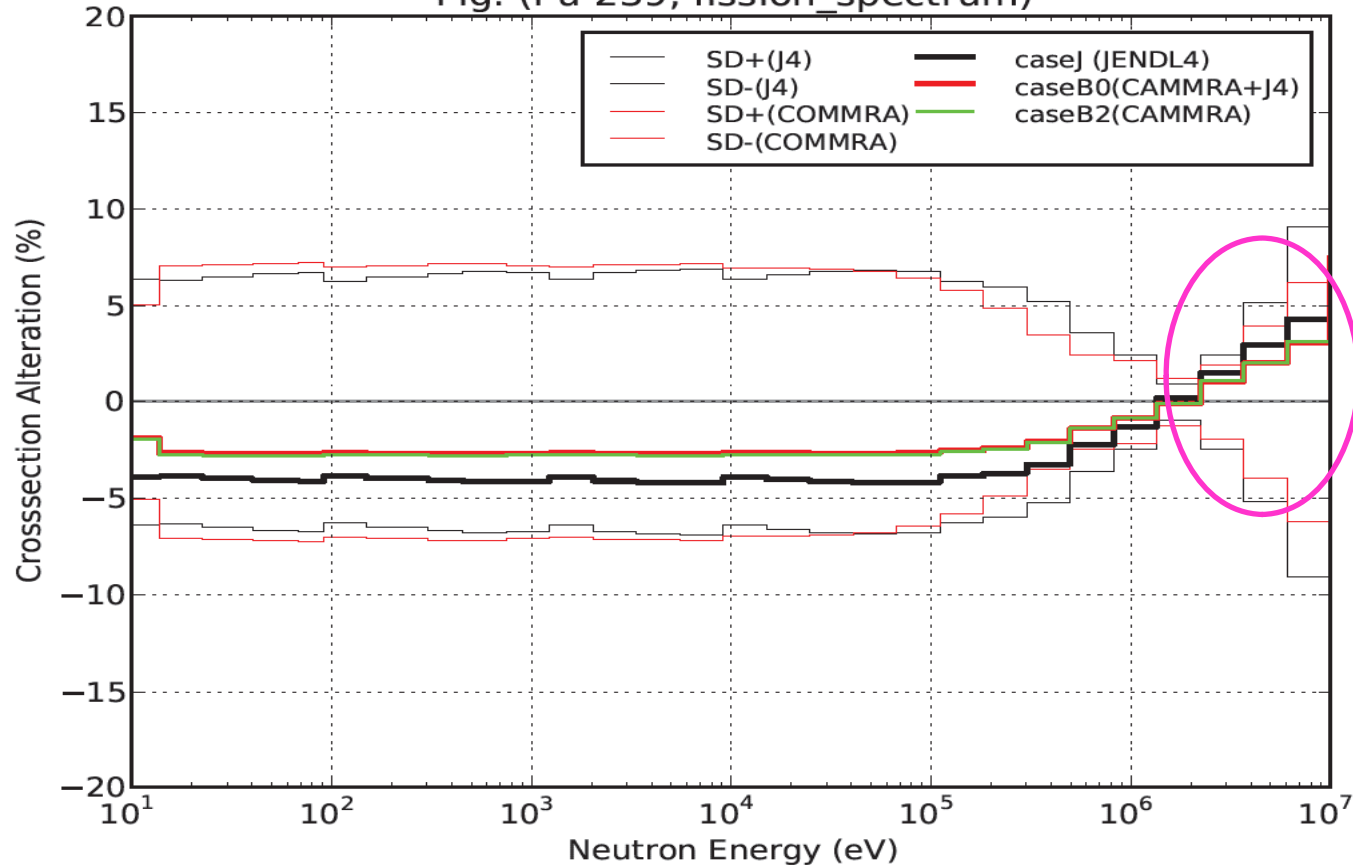


⇒ **Total C/E changes were identical between JENDL and COMMARA. In detail, there occurred a cancellation of Pu-239 chi and Fe-56 elastic scattering.**

Change of Nuclear data (1)

Pu-239: Fission spectrum

Fig. (Pu-239, fission_spectrum)

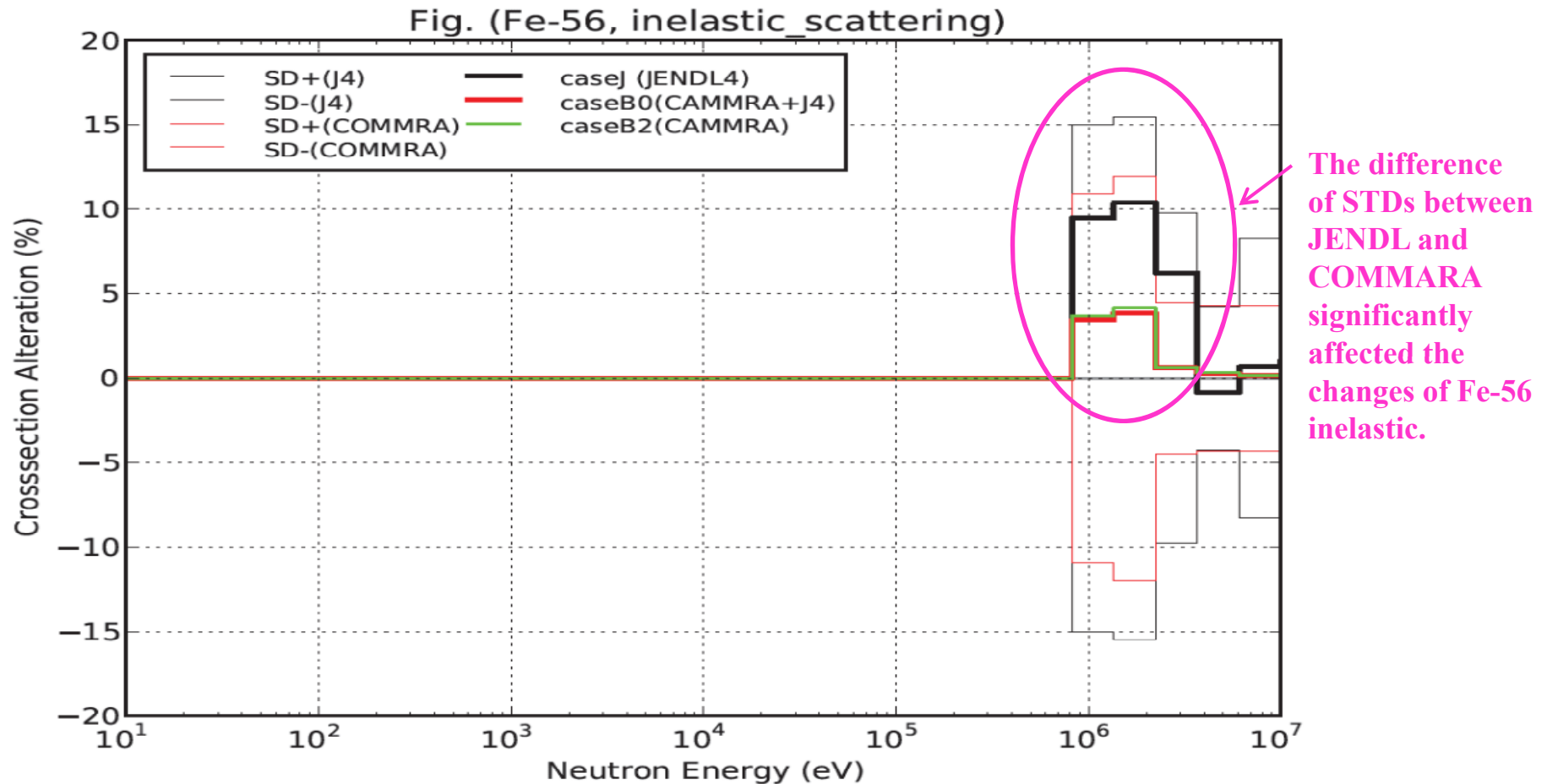


We need to find the mechanism of this Pu-239 chi change.

=> Flux spectrum was hardened, in spite of the opposite direction with keff C/E change.

Change of Nuclear data (2)

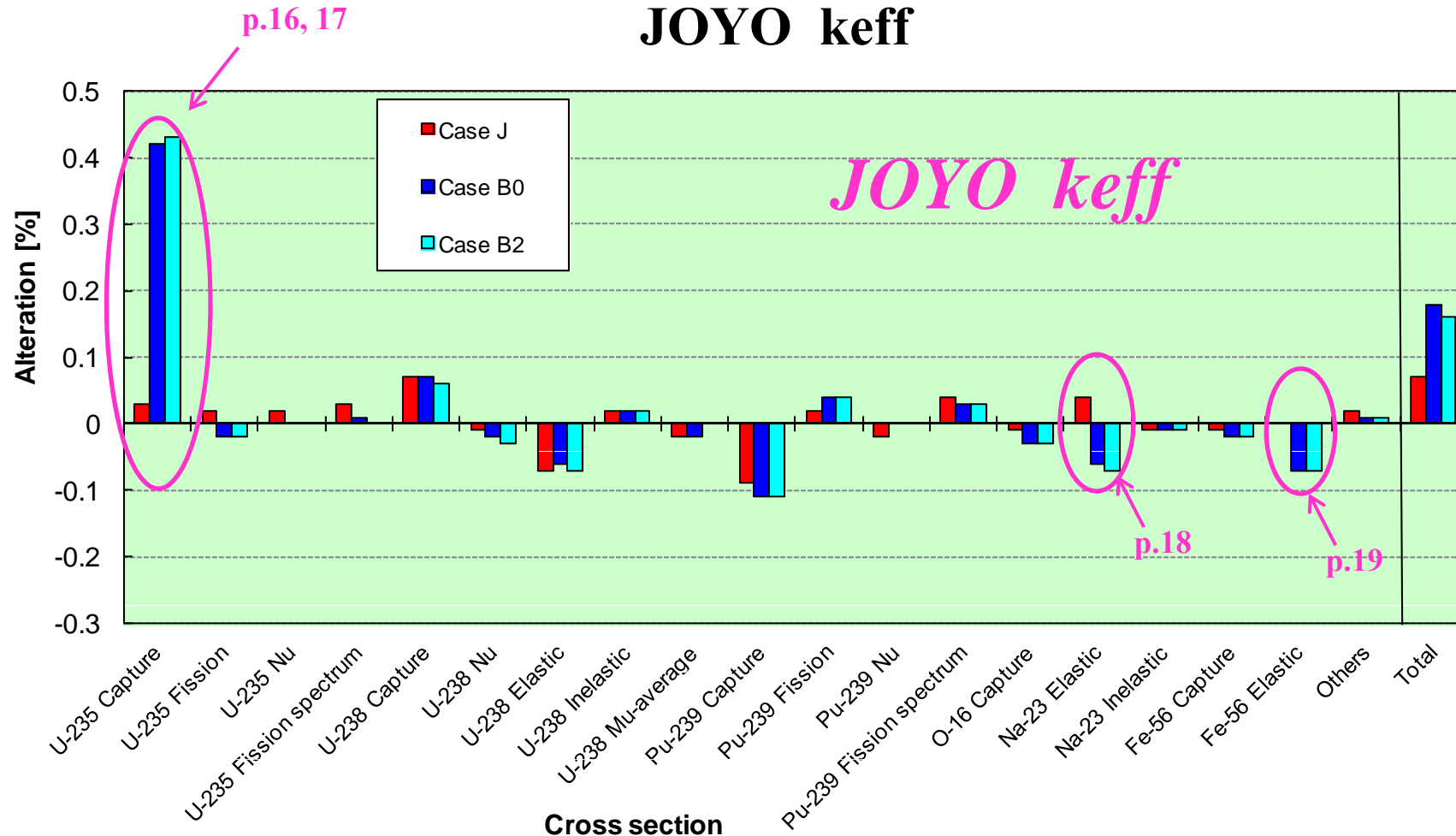
Fe-56: Inelastic



=> Flux spectrum was softened, which was consistent with keff C/E change.

Contribution to C/E change (2)

JOYO keff

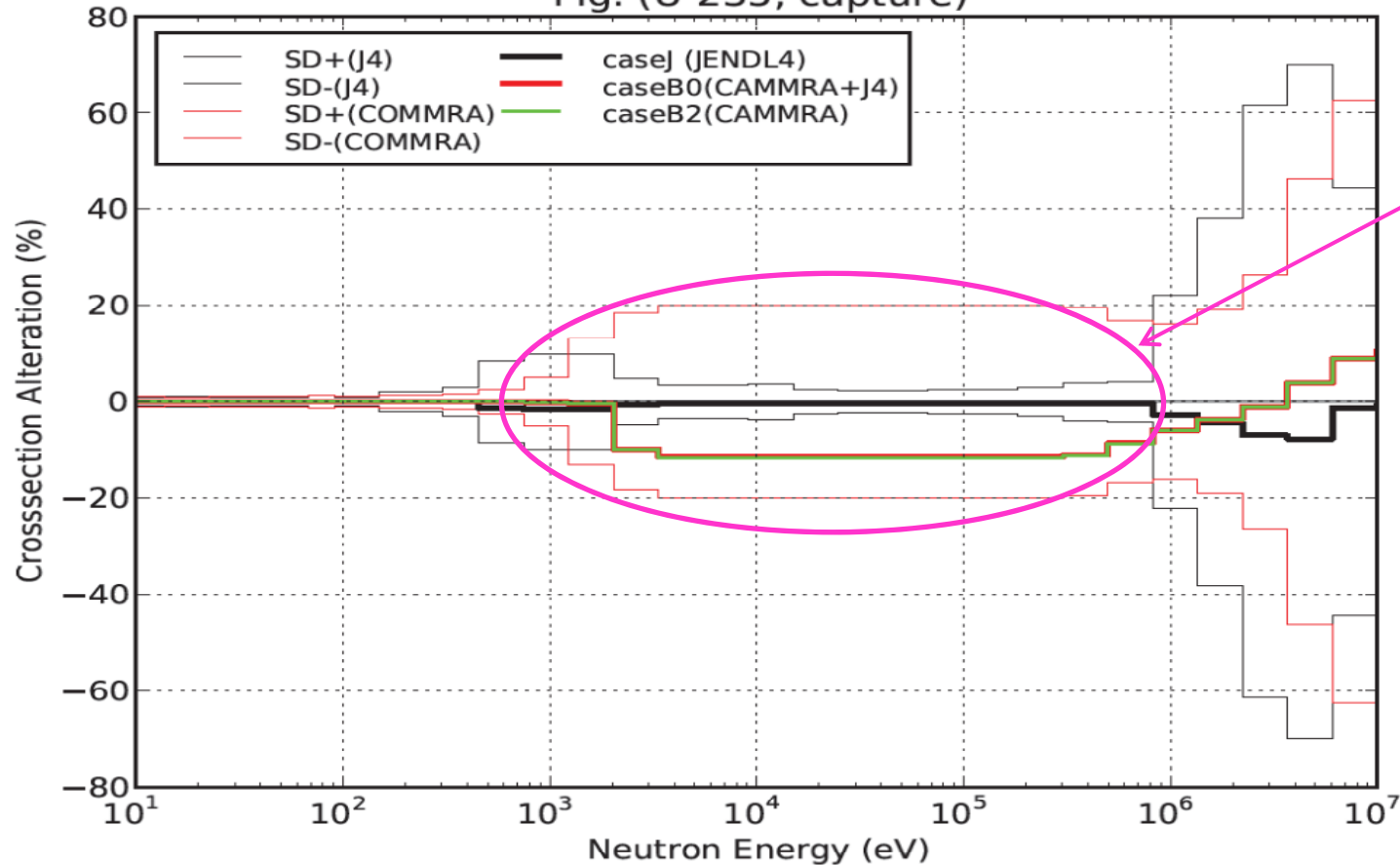


⇒ The contribution of U-235 capture were significantly different between JENDL and COMMARA. Further, those of Na-23 and Fe-56 elastic scattering were opposite in sign.

Change of Nuclear data (3)

U-235: Capture

Fig. (U-235, capture)



The difference of STDs between JENDL and COMMARA significantly affected the changes of U-235 capture.

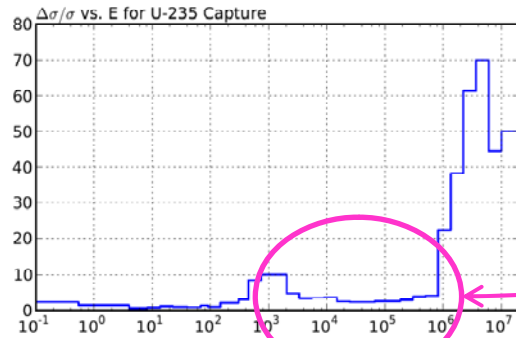
=> The change of COMMARA is consistent with the conclusion of SG-29, that is, the overestimation of U-235 capture in ENDF/B-7.

Comparison of Covariance (1)

U-235: Capture

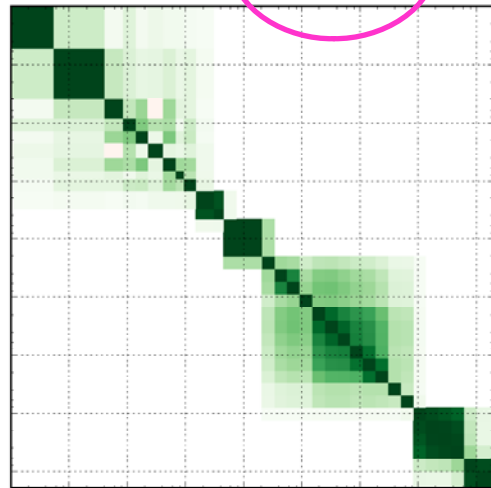
Fig. U-235 Capture

Fig. U-235 Capture

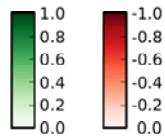


Ordinate scales are % relative standard deviation and barns.

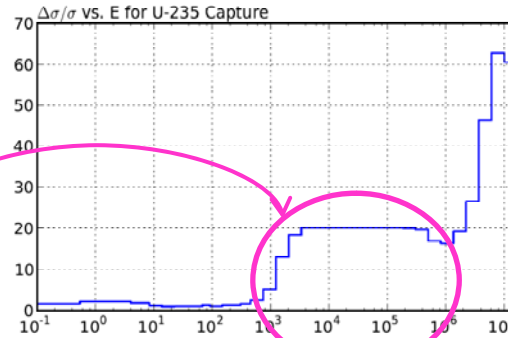
Abscissa scales are energy (eV).



Correlation Matrix

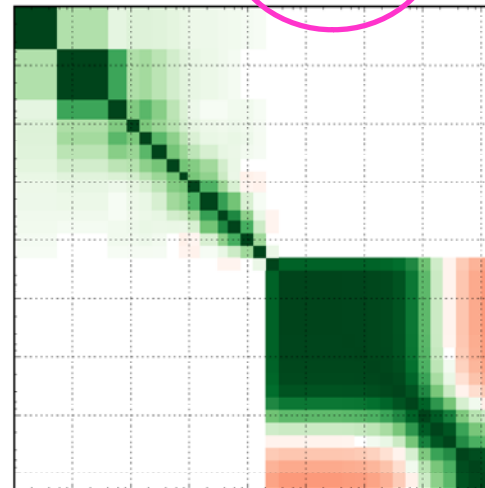


JENDL-4.0

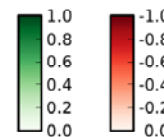


Ordinate scales are % relative standard deviation and barns.

Abscissa scales are energy (eV).



Correlation Matrix



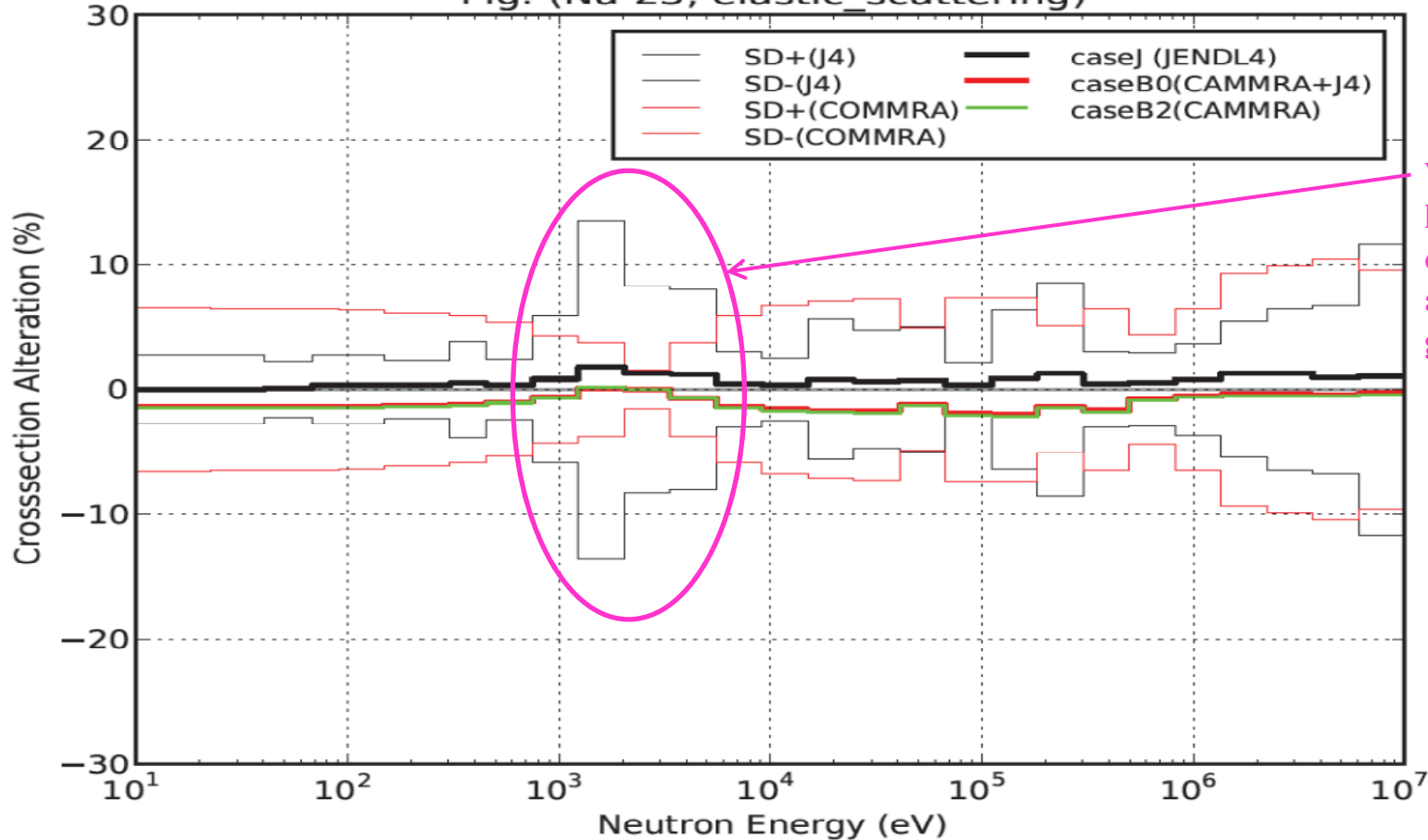
COMMARA 2.0



Change of Nuclear data (4)

Na-23: Elastic scattering

Fig. (Na-23, elastic_scattering)



Why did this large difference of STDs happen around the 2 keV giant resonance?

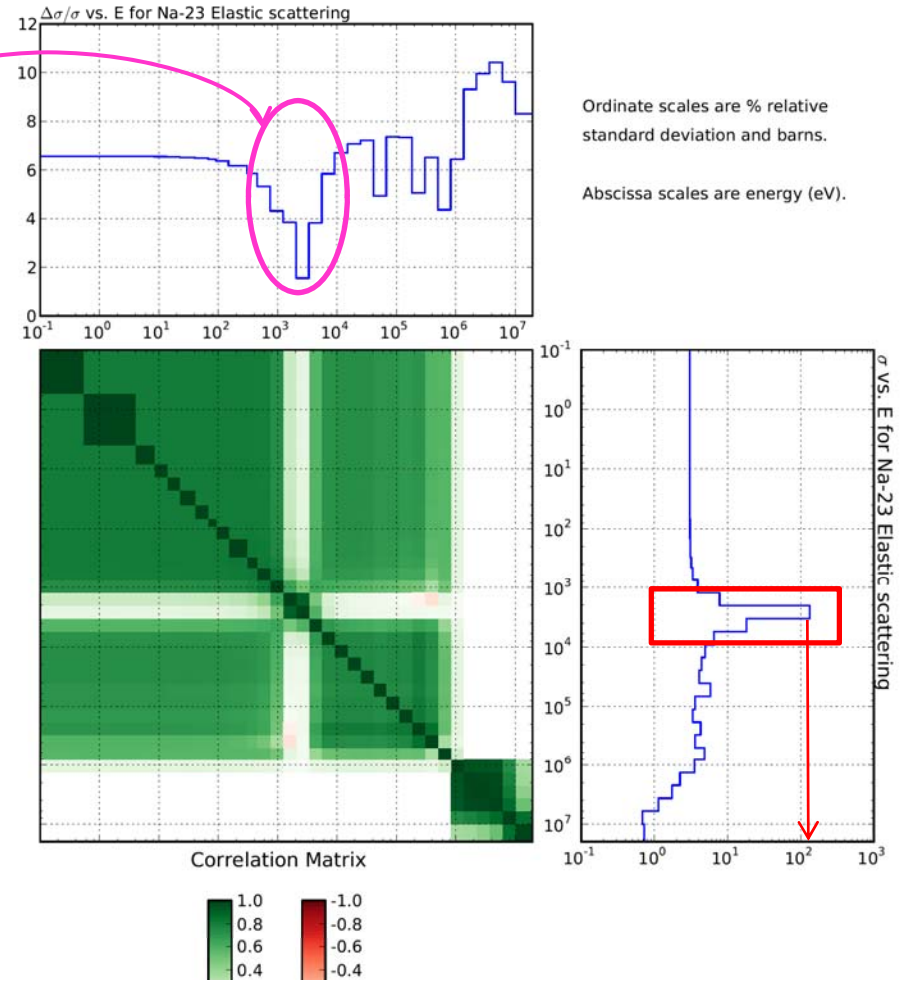
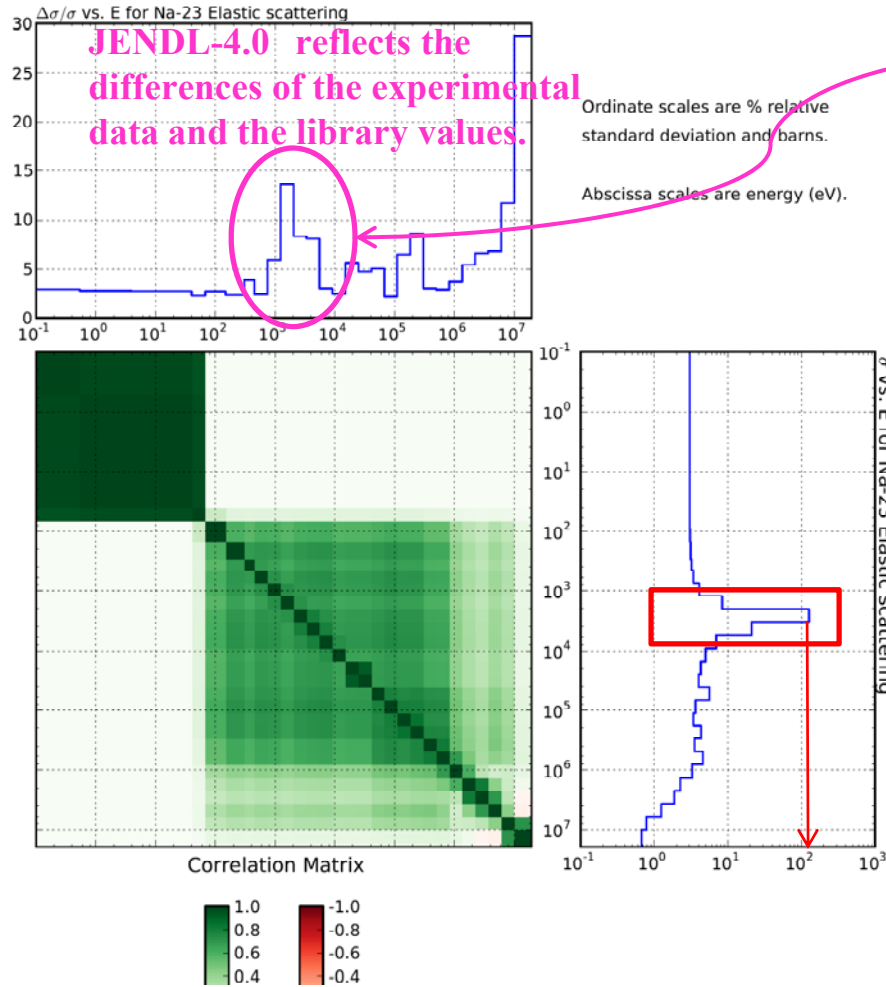
=> COMMARA increased the neutron leakage from JOYO core, i.e., the negative reactivity.

Comparison of Covariance (2)

Na-23: Elastic scattering

Fig. Na-23 Elastic scattering

Fig. Na-23 Elastic scattering



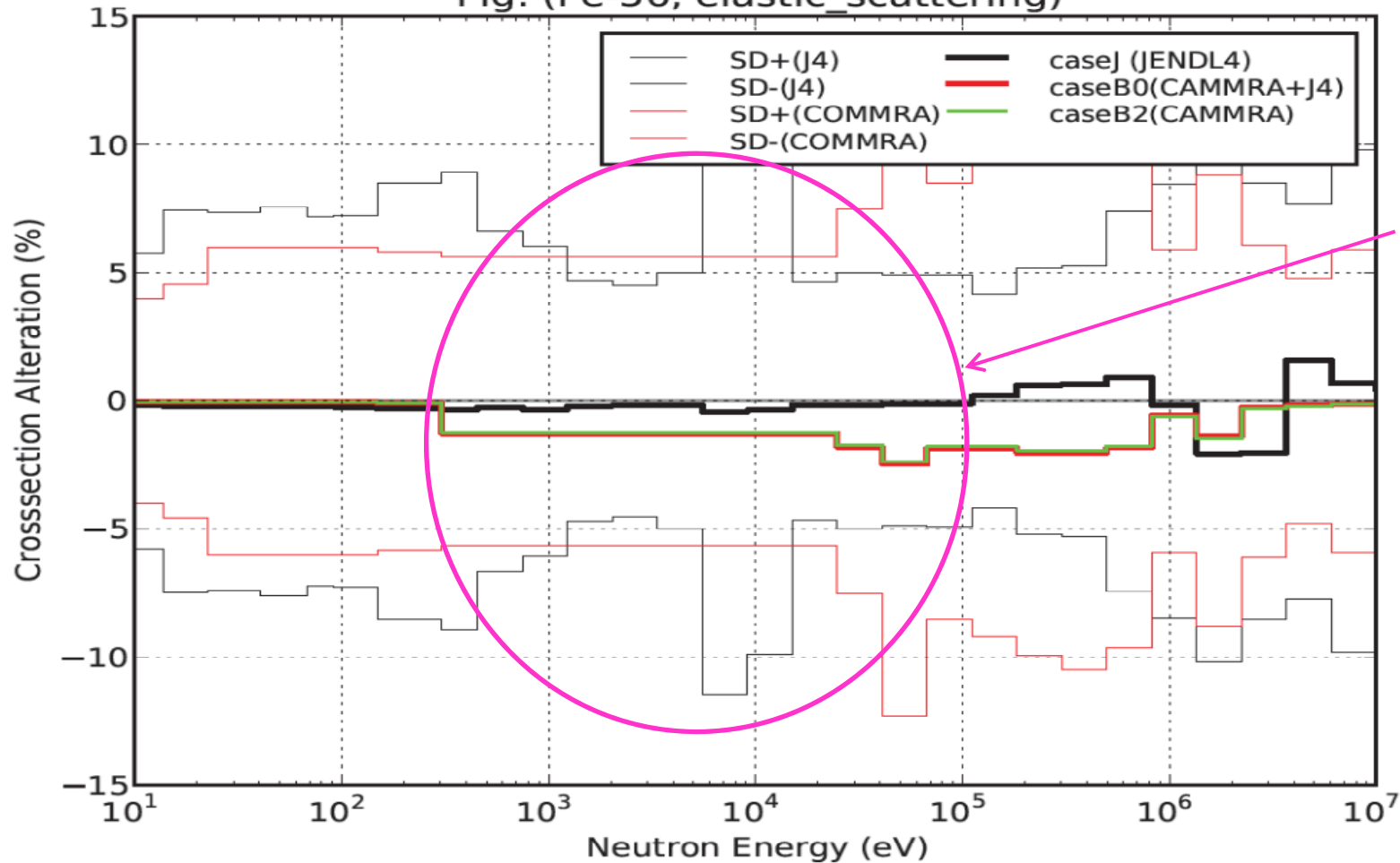
JENDL-4.0

COMMARA 2.0

Change of Nuclear data (5)

Fe-56: Elastic scattering

Fig. (Fe-56, elastic_scattering)



The difference of STDs between JENDL and COMMARA did not always affect the changes of Fe-56 elastic.

=> COMMARA increased the neutron leakage from JOYO core, i.e., the negative reactivity.

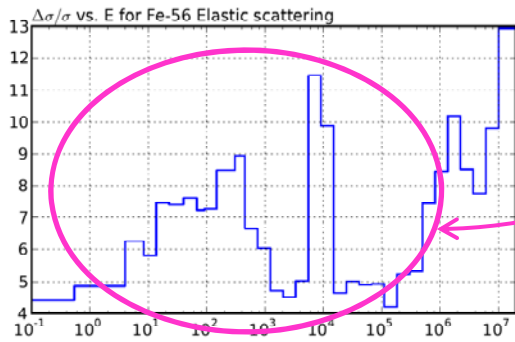


Comparison of Covariance (3)

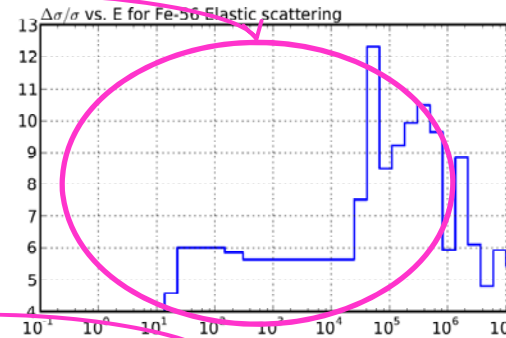
Fe-56: Elastic scattering

Fig. Fe-56 Elastic scattering

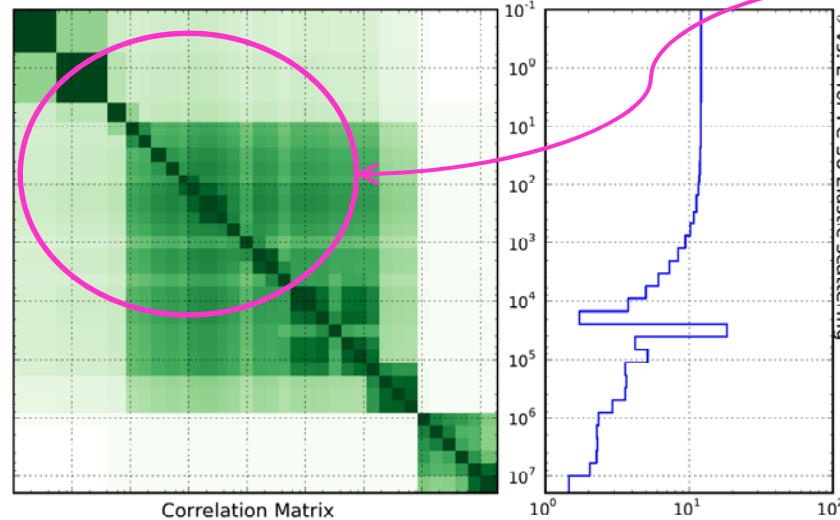
Fig. Fe-56 Elastic scattering



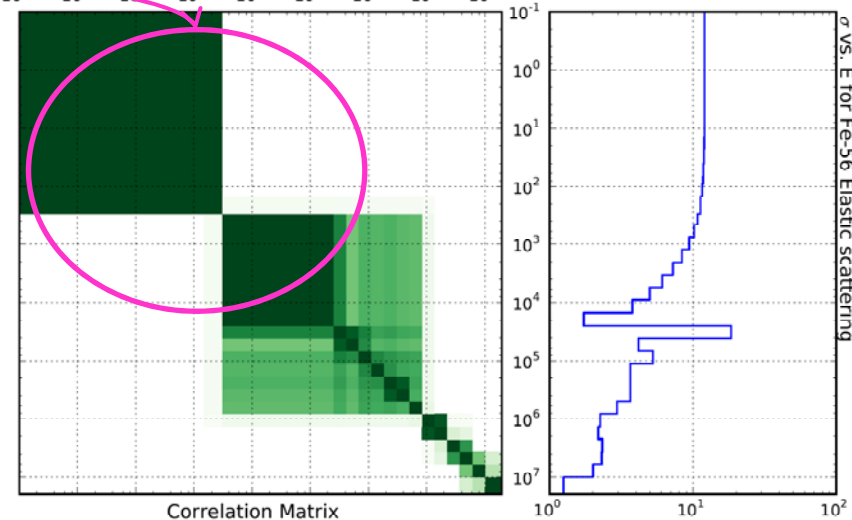
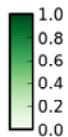
Ordinate scales are % relative standard deviation and bars.
Abscissa scales are energy (eV).



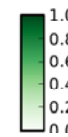
Ordinate scales are % relative standard deviation and bars.
Abscissa scales are energy (eV).



Correlation Matrix



Correlation Matrix



Why so different covariances for Fe-56 elastic between JENDL and COMMARA?

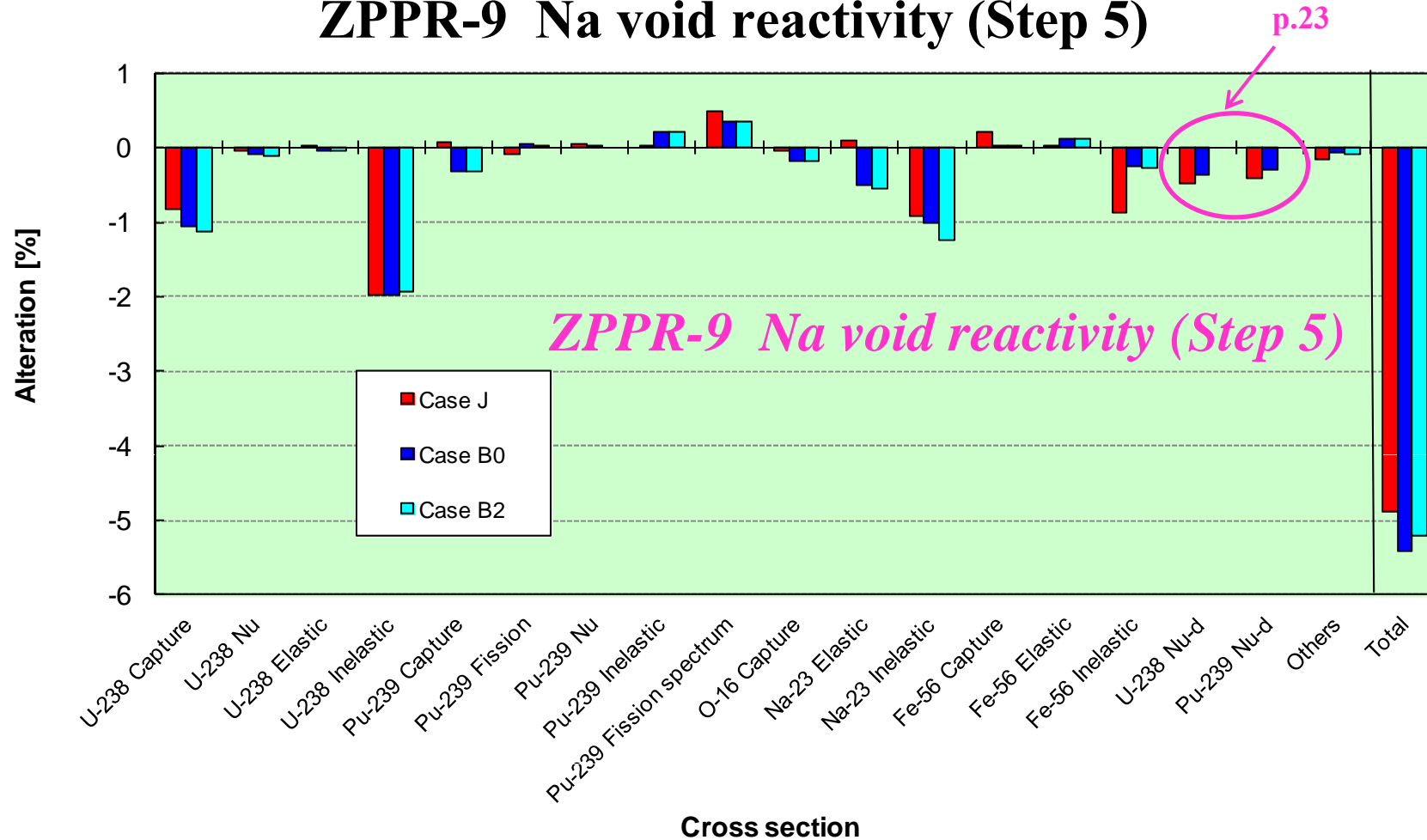
JENDL-4.0

COMMARA 2.0



Contribution to C/E change (3)

ZPPR-9 Na void reactivity (Step 5)



=> The effect of Nu-d appeared in the reactivity adjustment.

Change of nuclear data (6)

Delayed neutron fraction

Fission isotope	Standard deviation (%)	Change by adjustment		
		Case J	Case B0	Case B2
U-235	2.7 %	+0.00 %	+0.00 %	-
U-238	3.4 %	-0.49 %	-0.37 %	-
Pu-239	4.4 %	-0.41 %	-0.30 %	-
Pu-240	4.9 %	+0.00 %	+0.00 %	-
Pu-241	5.0 %	+0.00 %	+0.00 %	-

=> Nu-d should be included in the adjusted data. If we treat other reactivity data such as the control rod worth of ZPPR in the adjustment, the contribution will be quite important, since it was largely overestimated by both JENDL and ENDF in general.

Concluding Remarks

1. The adjusted C/E values were not significantly affected by the difference of covariance data between JENDL-4.0 and COMMAR 2.0.

→ *this can be expected from the basic equation in the appendix.*

2. On the other hand, the changes of nuclear data by the adjustment were extremely controlled by the covariance data, especially the standard deviation values.

→ *it will affect the extrapolation ability of the adjustment.*

3. (Proposal) As a part of SG33 activity, we should make the first conversation about the plausibility of covariance data, with nuclear data evaluators.

Appendix: Theory of Cross-section Adjustment

※ J.B.Dragt, et al.: “Methods of Adjustment and Error Evaluation of Neutron Capture Cross Sections; Application to Fission Product Nuclides,” NSE 62, pp.117-129, 1977

- Based on the Bayes theorem, i.e., the conditional probability estimation method
 → To maximize the posterior probability that a cross-section set, T , is true, under the condition that the information of integral experiment, Re , is obtained.

$$J(T) = (T-T_0)^t M^{-1} (T-T_0) + [Re-Rc(T)]^t [Ve+Vm]^{-1} [Re-Rc(T)]$$

Minimize the function $J(T)$. → $dJ(T)/dT = 0$

- The adjusted cross-section set T' , and its uncertainty (covariance), M' (Algebra)

$$T' = T_0 + MG^t [GMG^t + Ve + Vm]^{-1} [Re - Rc(T_0)]$$

$$M' = M - MG^t [GMG^t + Ve + Vm]^{-1} GM$$



✓ If $GMG^t \ll Ve + Vm$, $T' \doteq T_0$ and $GM'G^t \doteq GMG^t$
 ✓ If $GMG^t \gg Ve + Vm$, $GM'G^t \doteq Ve + Vm$
 ✓ If $GMG^t \doteq Ve + Vm$, $GM'G^t \doteq 1/2 \times GMG^t$

- Prediction error induced by the cross-section errors

Before adjustment: GMG^t

After adjustment: $GM'G^t$

Where, T_0 : Cross-section set before adjustment

Ve : Experimental errors of integral experiments

M : Covariance before adjustment

Vm : Analytical modeling errors of integral experiments

Re : Measured values of integral experiments

G : Sensitivity coefficients, $(dR/R)/(d\sigma/\sigma)$

Rc : Analytical values of integral experiments

