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CIELO-2 Based Cross-section Adjustment by Adding New Experiments on the Basis of the SG33 Benchmark

K. Yokoyama and M. Ishikawa

Japan Atomic Energy Agency

Acknowledgment: The authors express sincere thanks to Mr. T. Jin of NESI incorporation for his many helps of performing the adjustment calculations and pre- and post-processing the results for this presentation.

Background

- In the last SG39 meeting, JAEA presented updated results of JENDL-4.0 based cross-section adjustment on the basis of the SG33 benchmark so as to investigate the effect of addition of new integral experiments, such as SNEAK and PROTEUS

- After the last meeting, CIELO-2 files with covariance data were distributed to SG39 members (May 2017)

CIELO-2 based cross-section adjustment are performed with the SG33 benchmark and the PROTEUS and SNEAK data

CIELO-2 version used for this adjustment

- This adjustment was based on “CIELO2-to-SG39” package, which was provided from Dr. Cabellos to SG39 members on May 21, 2017.
- 11 evaluated files: 9 (JEFF-3.3T3) + 2 (JEFF-3.3T2- O16 & Fe56)
  - 5-B-10g.jeff33t3
  - 8-O-16g.jeff33t2
  - 11-Na-23g.jeff33t3
  - 24-CR-52g.jeff33t3
  - 26-Fe-56g.jeff33t2
  - 28-Ni-58g.jeff333t3
  - 92-U-235g.jeff33t3
  - 92-U-238g.jeff33t3
  - 94-Pu-239g.jeff33t3
  - 94-Pu-240g.jeff33t3
  - 94-Pu-241g.jeff33t3
- The above all files, including other than the CIELO targets (O-16, Fe-56, U-235, U-238, and Pu-239) are used for this adjustment.
- As for Pu-242, JENDL-4.0 is used instead of CIELO-2.

Integral Experiments of SG33 Benchmark

- JEZEBEL Pu-239:
  - KEFF, F28/F25, F49/F25, F37/F25
- JEZEBEL Pu-240:
  - KEFF
- FLATTOP-Pu:
  - KEFF, F28/F25, F37/F25
- ZPR6-7:
  - KEFF, F28/F25, F49/F25, C28/F25
- ZRR6-7 high Pu-240 content:
  - KEFF
- ZPPR-9:
  - KEFF, F28/F25, F49/F25, C28/F25, SVR(central void), SVR(leakage-dominant)
- JOYO:
  - KEFF

→ Total 20 integral experiments

New Integral Experiments provided by SG39

- PROTEUS
  - HCLWR-PROTEUS
    - Core 7: moderated by water (Vm/Vf=0.48)
      - KINF (k_∞), Void reactivity worth, C28/F49, F28/F49, F25/F49, F41/F49, C42/F49
    - Core 8: not moderated
      - KINF (k_∞), C28/F49, F28/F49, F25/F49, F41/F49, C42/F49
  - Code & Library
    - MCNP6.11 & JEFF-3.1.1
- SNEAK
  - MOX fuel reflected by metallic depleted uranium
    - 7A: PuO2-UO2, graphite
      - KEFF (k_{eff})
    - 7B: PuO2-UO2, ^{nat}UO2
      - KEFF (k_{eff})
  - Code & Library
    - THREEDANT & ENDF/B-VII.1

→ + 15 integral experiments

Input Data for Additional Integral Experiments

- C/E values
  - Calculated values with a nuclear data library, x, are converted into those with CIELO-2 by using sensitivity coefficients:

$$C_{CIELO-2} = C_x \times \left(1 + S_x \frac{\sigma_{CIELO-2} - \sigma_x}{\sigma_x} \right)$$

- Sensitivity coefficients
  - Given 33-group sensitivity coefficients are used without any modifications because the sensitivity coefficients are less sensitive to the nuclear data libraries
- Uncertainty and correlation
  - Experimental uncertainty :
    - Given data are used as they are
  - Analytical model uncertainty :
    - Ignored (set to zero)
  - Correlation factor:
    - Correlation factors between the other experiments are set to zero
    - Correlation factors for spectral indices of PROTEUS are tentatively set to 0.5
      - All reaction rate ratios have the same denominator (F49)

C/E Values of HCLWR-PROTEUS

Table: C/E and experimental uncertainty for PROTEUS Core7 and 8

		C/E* (JEFF-3.1.1)	C/E (JENDL-4.0)	Chi	C/E (CIELO-2)	Chi	Rejected
Core 7	Kinf	1.008±0.006	1.0123	1.30	1.0119	0.93	
Core 8	Kinf	0.996±0.004	0.9993	0.06	1.0043	0.35	
Core 7/8	Void reactivity	0.78±0.11	0.7048	0.38	2.4486	1.69	✓
Core 7	C28/F49	1.012±0.018	1.0095	0.42	0.9834	0.72	
	F28/F49	1.006±0.019	1.0169	0.38	0.9938	0.15	
	F25/F49	1.015±0.015	1.0109	0.65	1.0146	0.55	
	F41/F49	0.988±0.030	0.9814	0.53	0.9626	1.01	
	C42/F49	1.024±0.031	1.0137	0.36	0.9909	0.27	
Core 8	C28/F49	1.021±0.016	1.0099	0.42	0.9828	0.70	
	F28/F49	0.984±0.018	0.9939	0.10	0.9620	1.05	
	F25/F49	1.025±0.013	1.0015	0.09	1.0189	0.39	
	F41/F49	1.022±0.031	0.9970	0.09	0.9989	0.03	
	C42/F49	1.229±0.037	1.1664	1.77	1.1741	5.26	✓

*: M. Hursin, et al., “Description of the Data provided to the SG39 with respect to the HCLWR experiments at Proteus,” AN-41-15-05 V.1, PSI (Dec. 19, 2016)

C/E values of SNEAK-7A/-7B

Table: C/E and experimental uncertainty for SNEAK-7A/-7B

	C/E* (ENDF/B-VII.1)	C/E (JENDL-4.0)	Chi	C/E (CIELO-2)	Chi	Rejected
SNEAK-7A KEFF	1.0054±0.0029	1.0109	1.45	1.0114	0.86	
SNEAK-7B KEFF	1.0042±0.0035	1.0098	0.99	1.0120	0.92	

I. Kodeli, "Sensitivities profiles: Flattop-Pu, SNEAK-7A, SNEAK-7B, ASPIS-FE88," WPEC/SG39 website, https://www.oecd-nea.org/science/wpec/sg39/

Sensitivity Coefficients

Adjusted nuclides and reactions		SNEAK 7A & 7B	PROTEUS 7 & 8
U-235	capture	●	●
	fission	●	●
	nu	●	●
	elastic_scattering	●	●
	inelastic_scattering	●	●
	fission_spectrum	●	●
U-238	capture	●	●
	fission	●	●
	nu	●	●
	elastic_scattering	●	●
	inelastic_scattering	●	●
	mu_average	●	●
	fission_spectrum	●	●
Pu-239	capture	●	●
	fission	●	●
	nu	●	●
	elastic_scattering	●	●
	inelastic_scattering	●	●
	mu_average	●	●
	fission_spectrum	●	●
Pu-240	capture	●	●
	fission	●	●
	nu	●	●
	elastic_scattering	●	●
	inelastic_scattering	●	●
	fission_spectrum	●	●
Pu-241	capture	●	●
	fission	●	●
	nu	●	●
	elastic_scattering	●	●
	inelastic_scattering	●	●
	fission_spectrum	●	●
Pu-242	capture	●	●
	fission	●	●
	nu	●	●
	elastic_scattering	●	●
	inelastic_scattering	●	●
	fission_spectrum	●	●

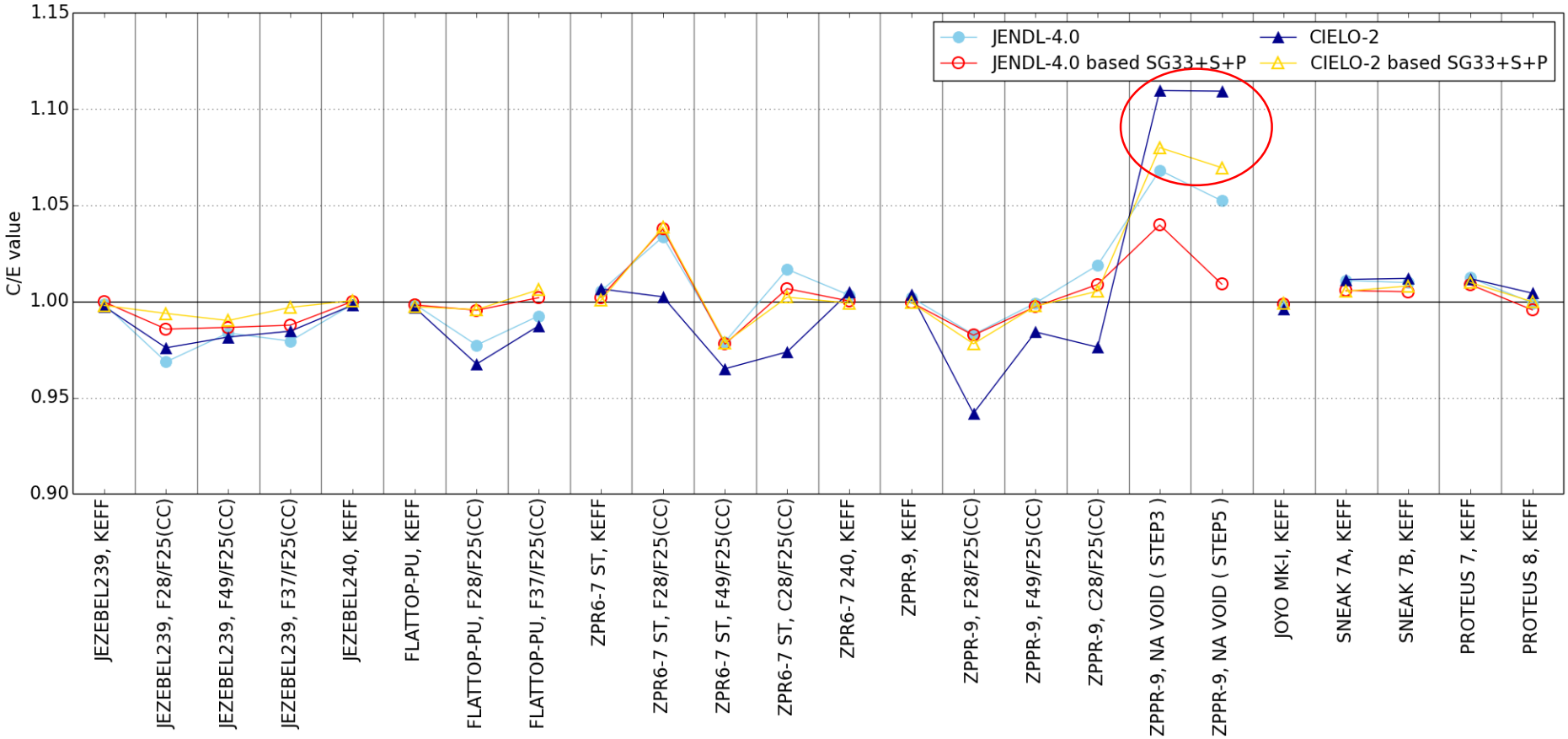
Adjusted nuclides and reactions		SNEAK 7A & 7B	PROTEUS 7 & 8
B-10	capture	---	●
	elastic_scattering	---	●
	inelastic_scattering	---	●
C-12	capture		---
	elastic_scattering		---
	inelastic_scattering		---
O-16	capture	●	●
	elastic_scattering	●	●
	inelastic_scattering	●	●
	mu_average		●
Na-23	capture	---	●
	elastic_scattering	---	●
	inelastic_scattering	---	●
Cr-52	capture		●
	elastic_scattering		●
	inelastic_scattering		●
	mu_average		●
Fe-56	capture	●	●
	elastic_scattering	●	●
	inelastic_scattering	●	●
	mu_average	●	●
Ni-58	capture		●
	elastic_scattering		●
	inelastic_scattering		●
	mu_average		●

- For PROTEUS, important sensitivity coefficients are fully included.
- For SNEAK, sensitivity coefficients of C-12, Cr-52 and Ni-58 are missing but they should be unimportant.

Case names

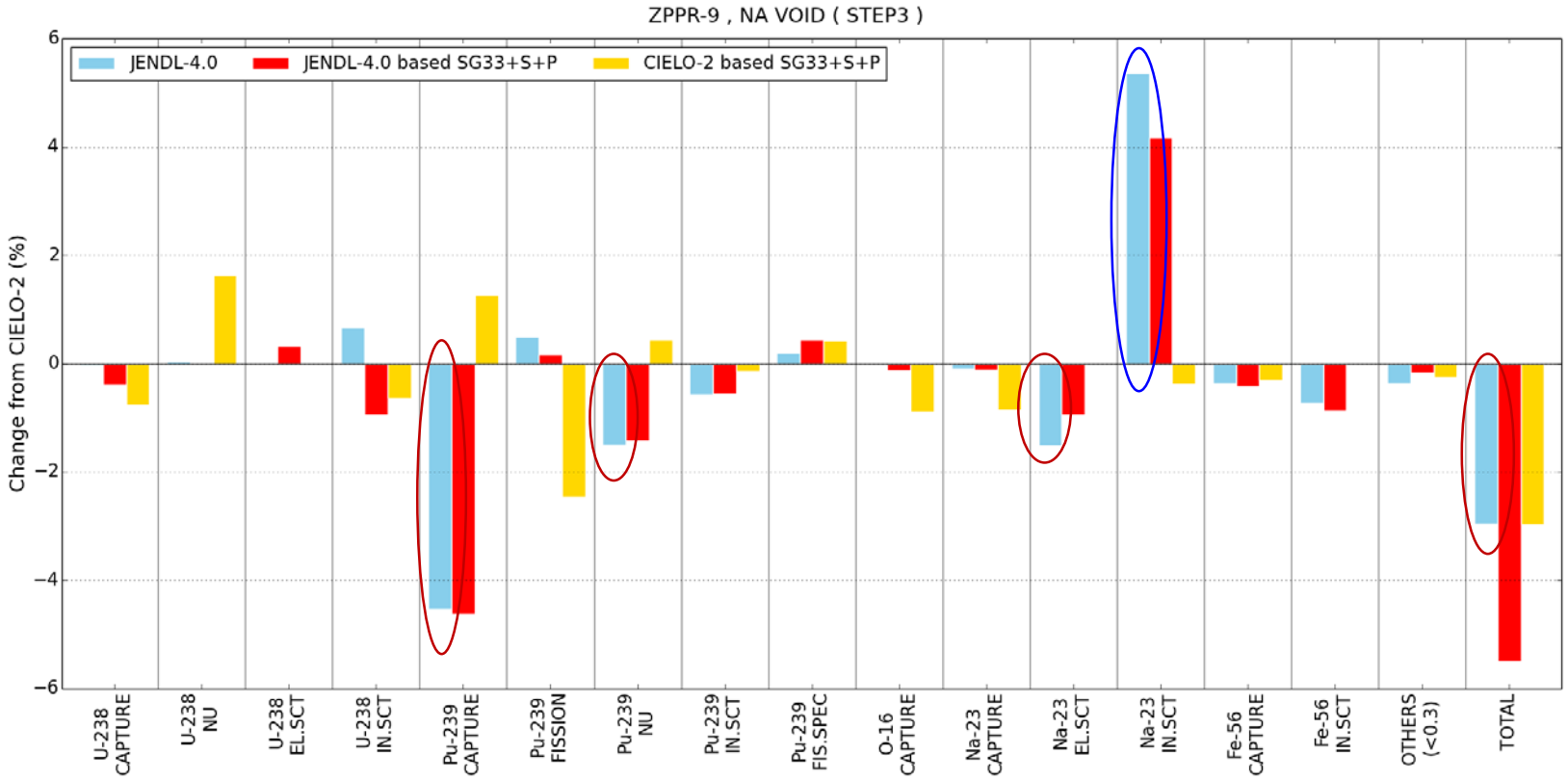
- Case1: “JENDL-4.0”
  - Results with the original (unadjusted) JENDL-4.0
- Case2: “JENDL-4.0 based SG33+S+P”
  - Adjustment results by adding both “SNEAK” and “PROTEUS” data to the SG33 benchmark dataset
- Case3: “CIELO-2”
  - Results with the original (unadjusted) CIELO-2
- Case4: “CIELO-2 based SG33+S+P”
  - Adjustment results by adding both “SNEAK” and “PROTEUS” data to the SG33 benchmark dataset

(1)-1 Overview of C/E values



- C/E values for both CIELO-2 and JENDL-4.0 look good in general.
- However, C/E values of ZPPR-9 sodium void reactivity (SVR) for CIELO-2 are very high (C/E > 1.1).

(1)-2 SVR: Contributions to ZPPR-9 step3 void



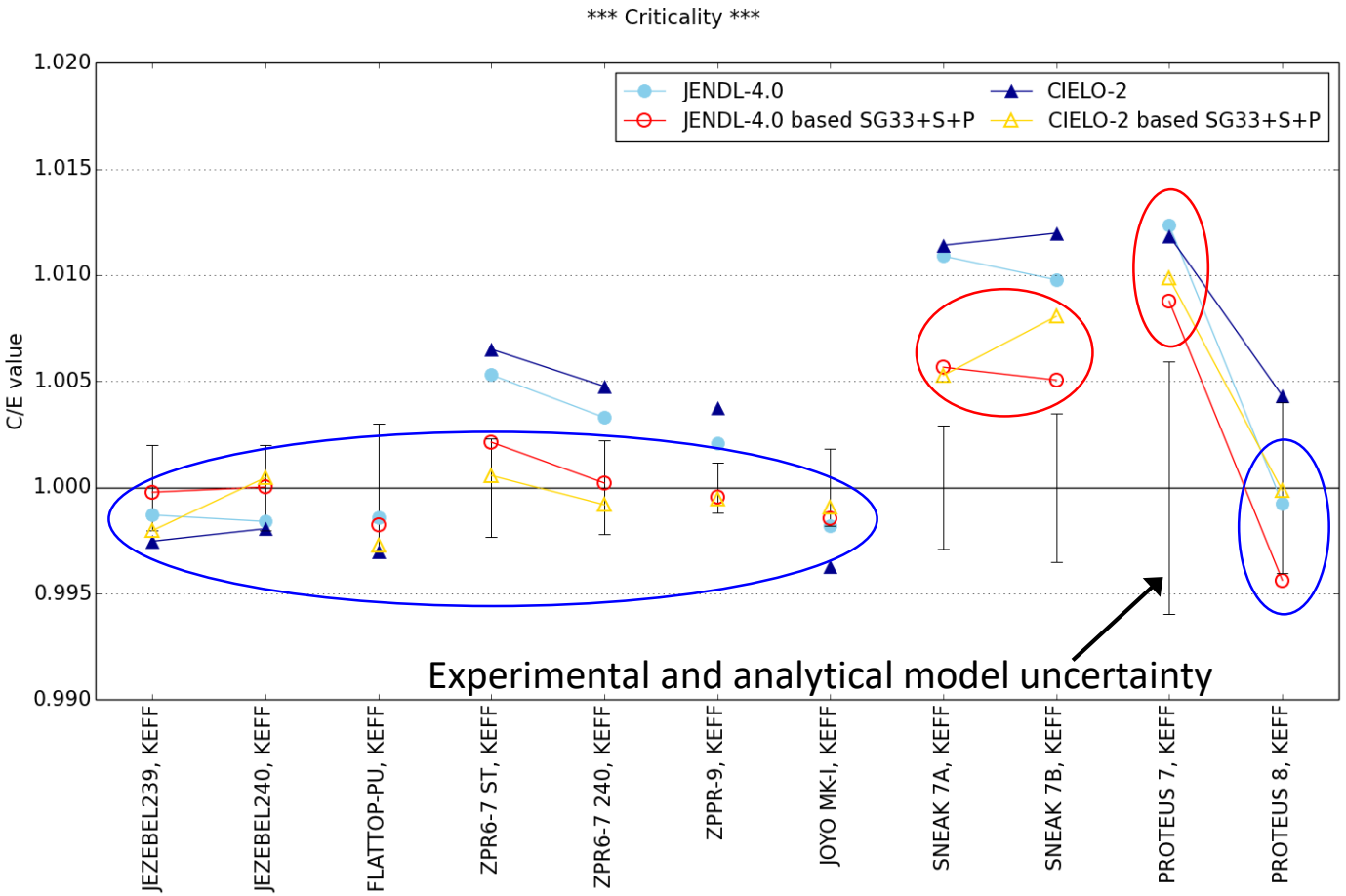
- Pu-239 capture, nu-bar, and Na-23 elastic of CIELO-2 worsen the C/E value of ZPPR-9 SVR in comparison with JENDL-4.0.
- On the other hand, the contribution of Na-23 inelastic is quite different between CIELO-2 and JENDL-4.0. If CIELO-2 adopts Na-23 inelastic of JENDL-4.0, C/E values of CIELO-2 will be much larger.

Summary (1)

- In CILEO-2, C/E values of ZPPR-9 sodium void reactivity (SVR) are not good (C/E > 1.1).

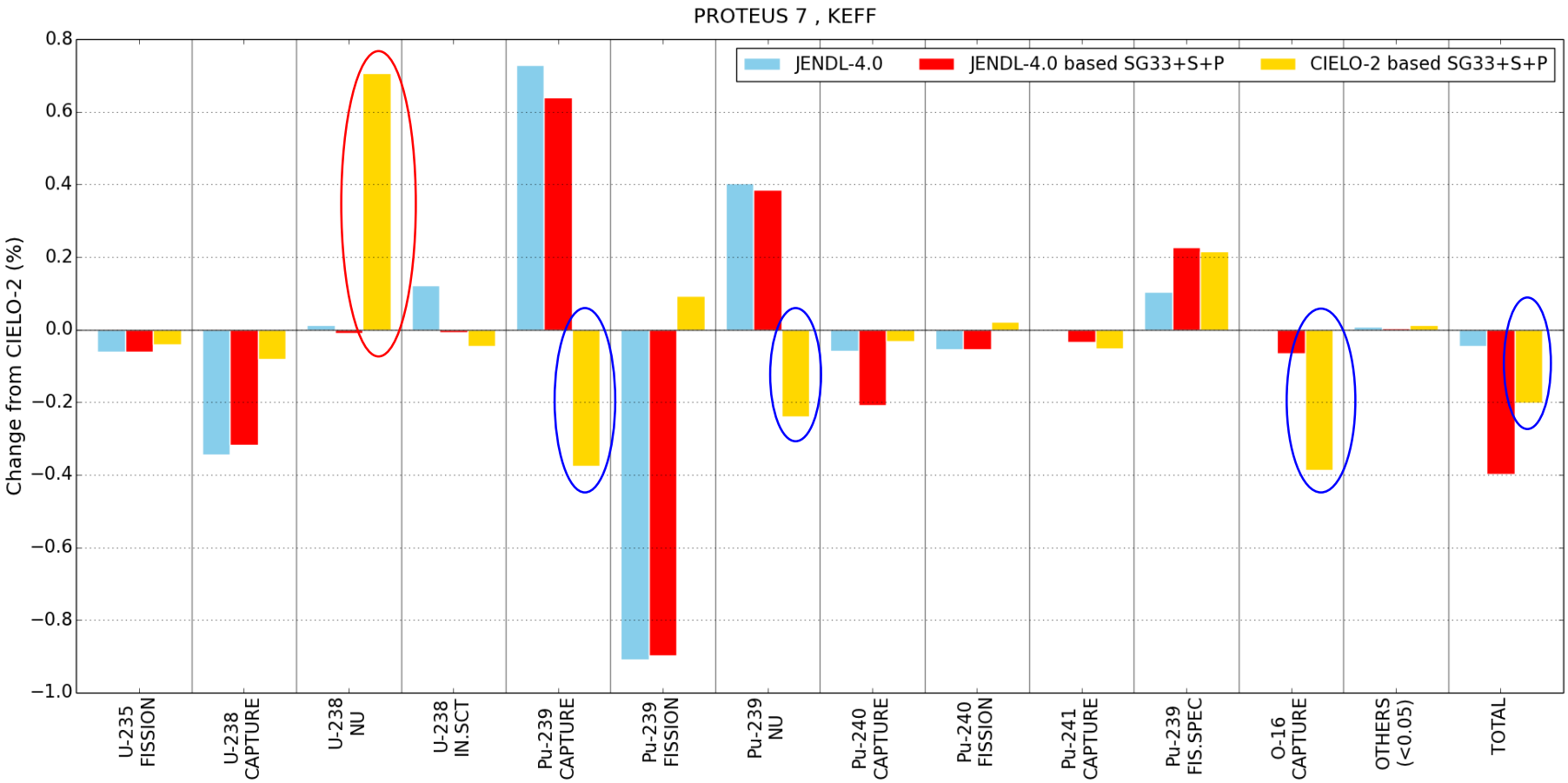
- Moreover, the C/E values of SVR are not improved well by adjustment.

(2)-1 Criticality: Overview of C/E values



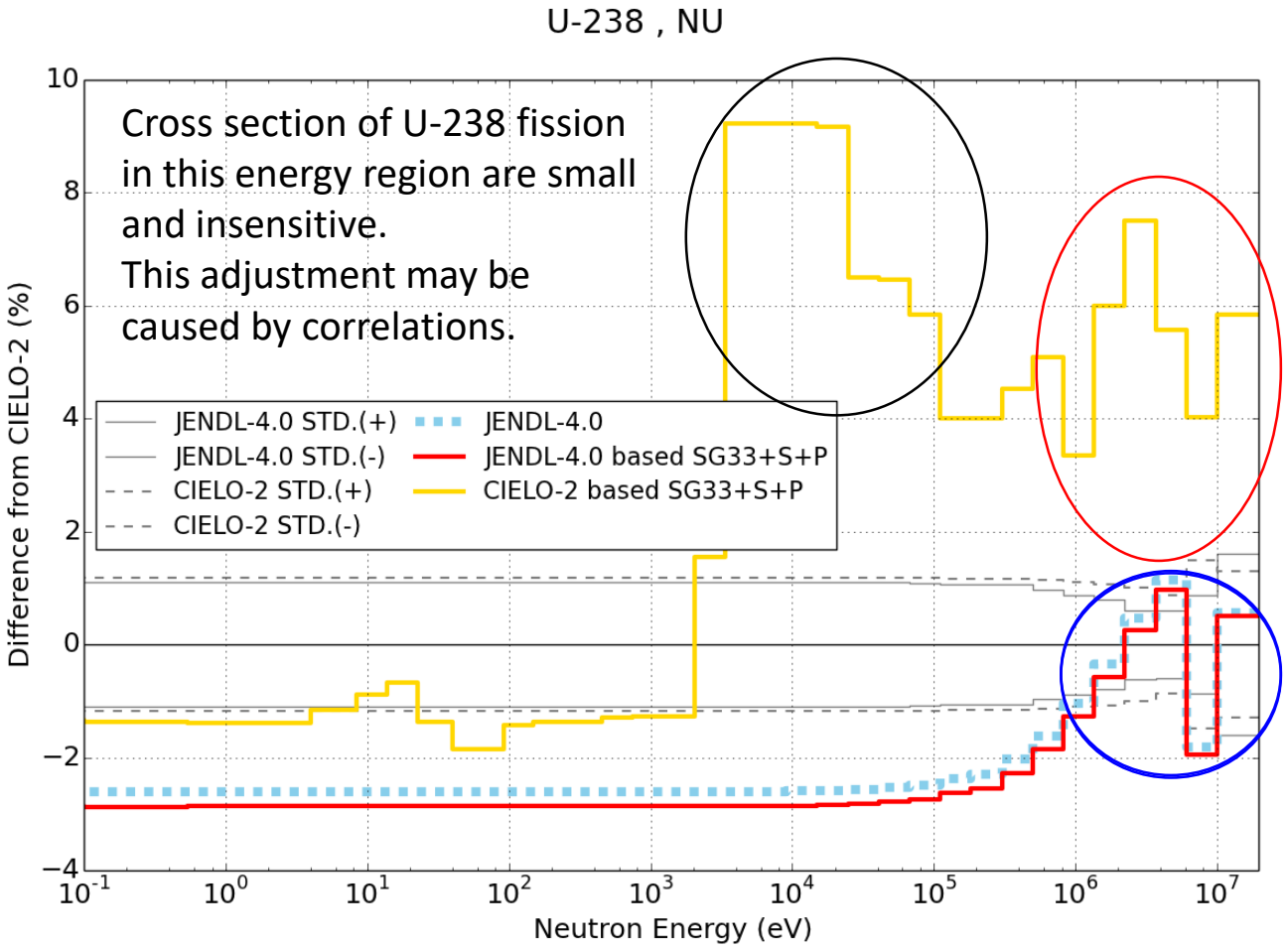
- Generally, C/E values are improved by adjustment both for JENDL-4.0 and CIELO-2.
- However, C/E values of SNEAK-7A, -7B, and PROTEUS 7 are not improved well.

(2)-2 Criticality: Contributions to PROTEUS 7



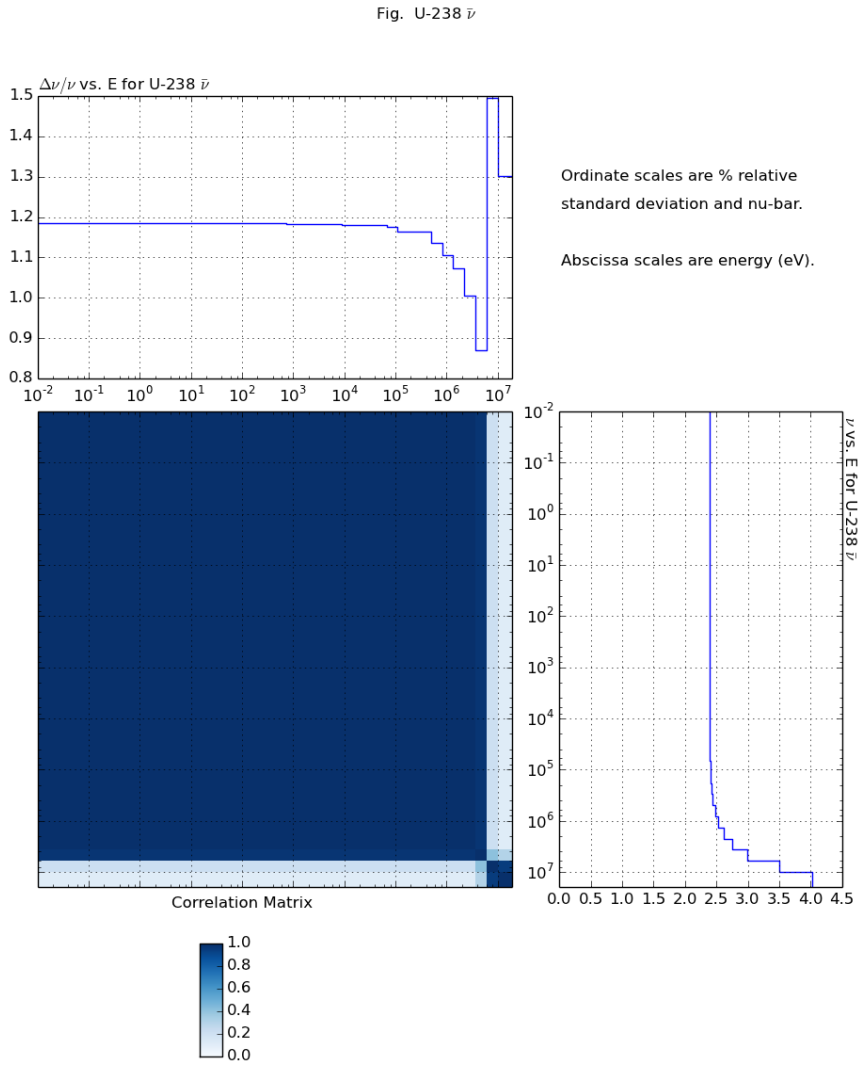
- In CIELO-2, the adjustments of Pu-239 capture, nu-bar, and O-16 capture improve C/E values of PROTEUS 7.
- However, the adjustment of U-238 nu-bar has a large inverse contribution.

(2)-3 Adjustment of U-238 nu-bar



- In CIELO-2, U-238 nu-bar was changed by adjustment exceeding 1-sigma uncertainty in the effective energy region (>1MeV).
- In JENDL-4.0, the adjustment of U-238 nu-bar was within 1-sigma uncertainty.

(2)-4 Covariance of U-238 nu-bar



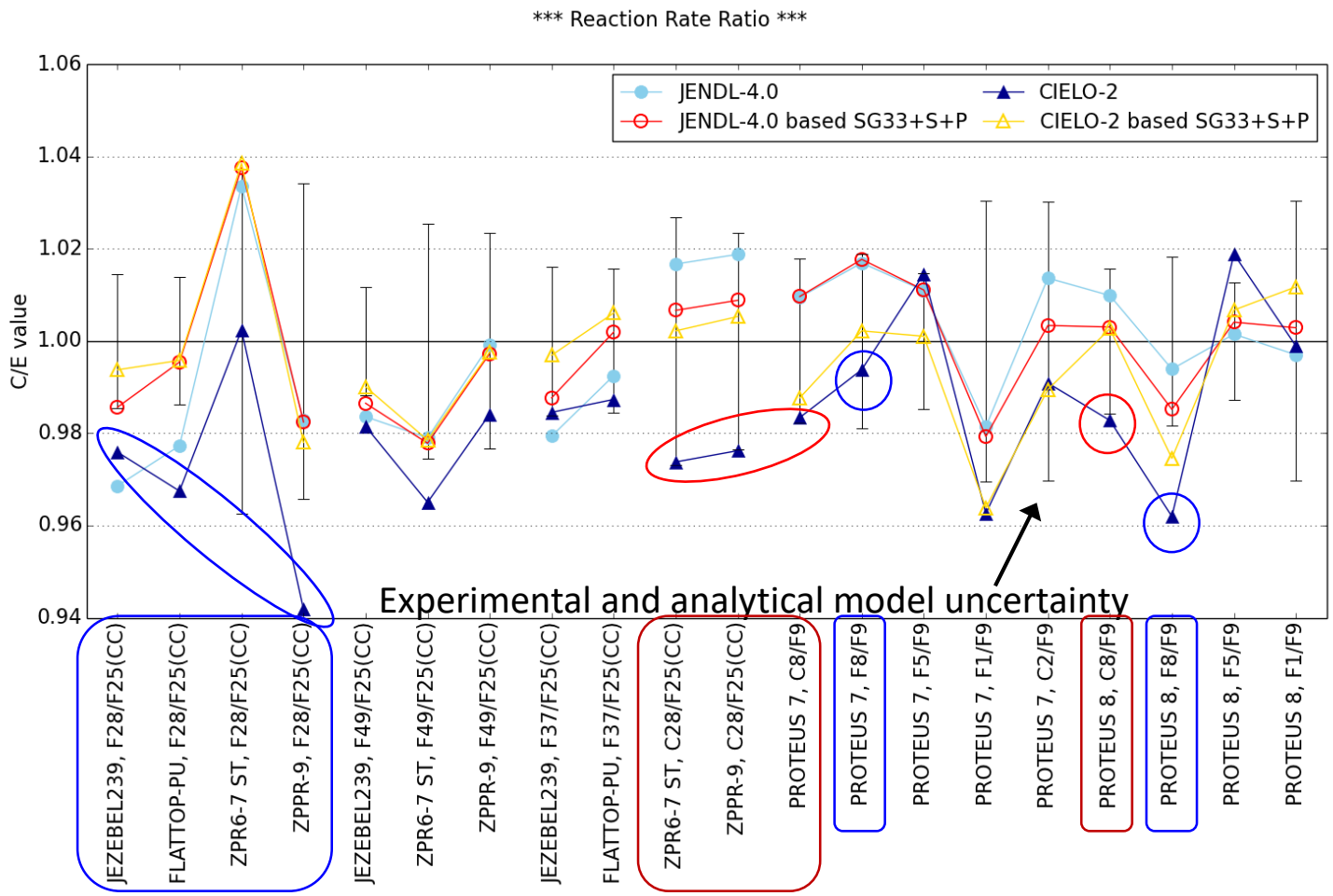
- In CIELO, U-238 nu-bar has very strong inter-energy correlations.
- These correlations cause the big change of U-238 nu-bar in 2keV -- 100keV.
- However, since U-238 nu-bar has similar strong inter-energy correlations in JENDL-4.0, this is NOT a specific problem in CIELO-2.

(2)-5 Why U-238 nu-bar is so largely adjusted

Adjustment cases	Change of 4th group () nu-bar of U-238 (STD: 1.0%)
SG33+s+p	7.5%
SG33+s+p without PROTEUS RRRs	6.2%
SG33+s+p without PROTEUS keffs	6.0%
SG33+s+p without SNEAK keffs	4.3%
SG33	3.6%
SG33+s+p without C28 RRRs	5.2%
SG33+s+p without F28 RRRs	4.9%

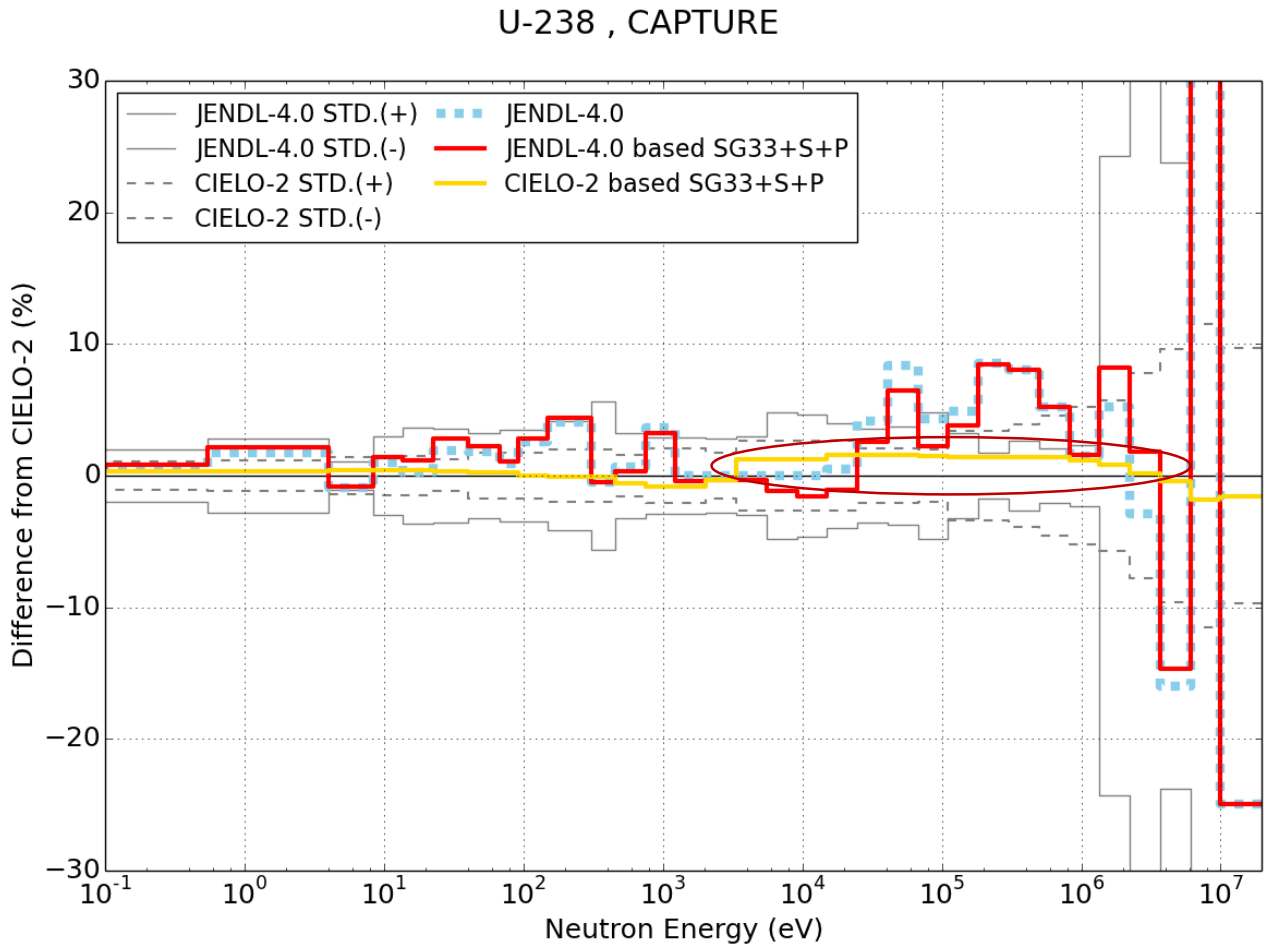
- If we remove criticalities of SNEAK, the amount of adjustment of U-238 nu-bar becomes smaller.
- On the other hand, we have a similar result when we remove all C28 or F28 RRRs

(2)-6 RRR: Overview of C/E values



- In CIELO-2, U-238 capture cross section (C28) should be enlarged for C/E values of C28 RRRs.
- In CIELO-2, U-238 fission cross section (F28) should be enlarged for C/E values of F28 RRRs.

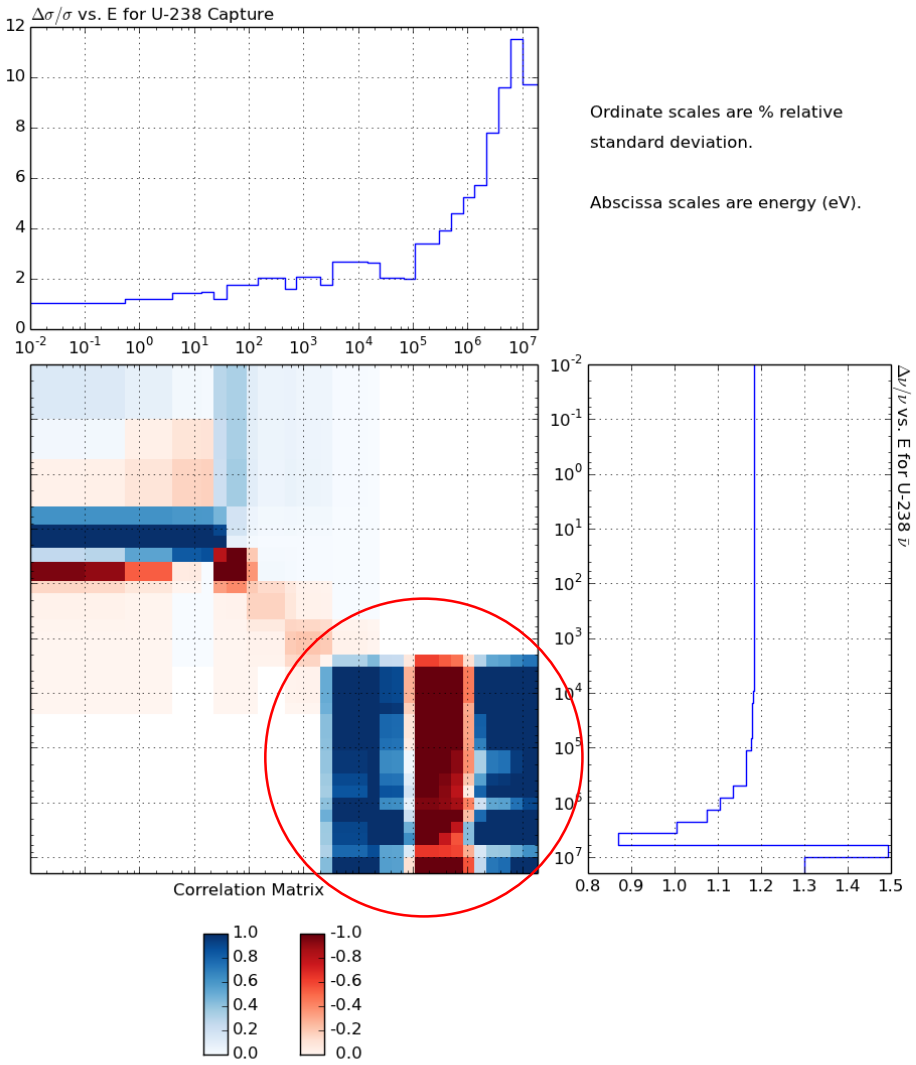
(2)-5 Adjustment of U-238 capture



- In CIELO-2, U-238 capture was enlarged by adjustment as expected from the C/E values of C28 RRRs.
- This adjustment reduces the C/E values of criticality. This is also a good news for criticalities of SNEAK & PROTEUS.

(2)-6 Correlation of U-238 capture vs. nu-bar

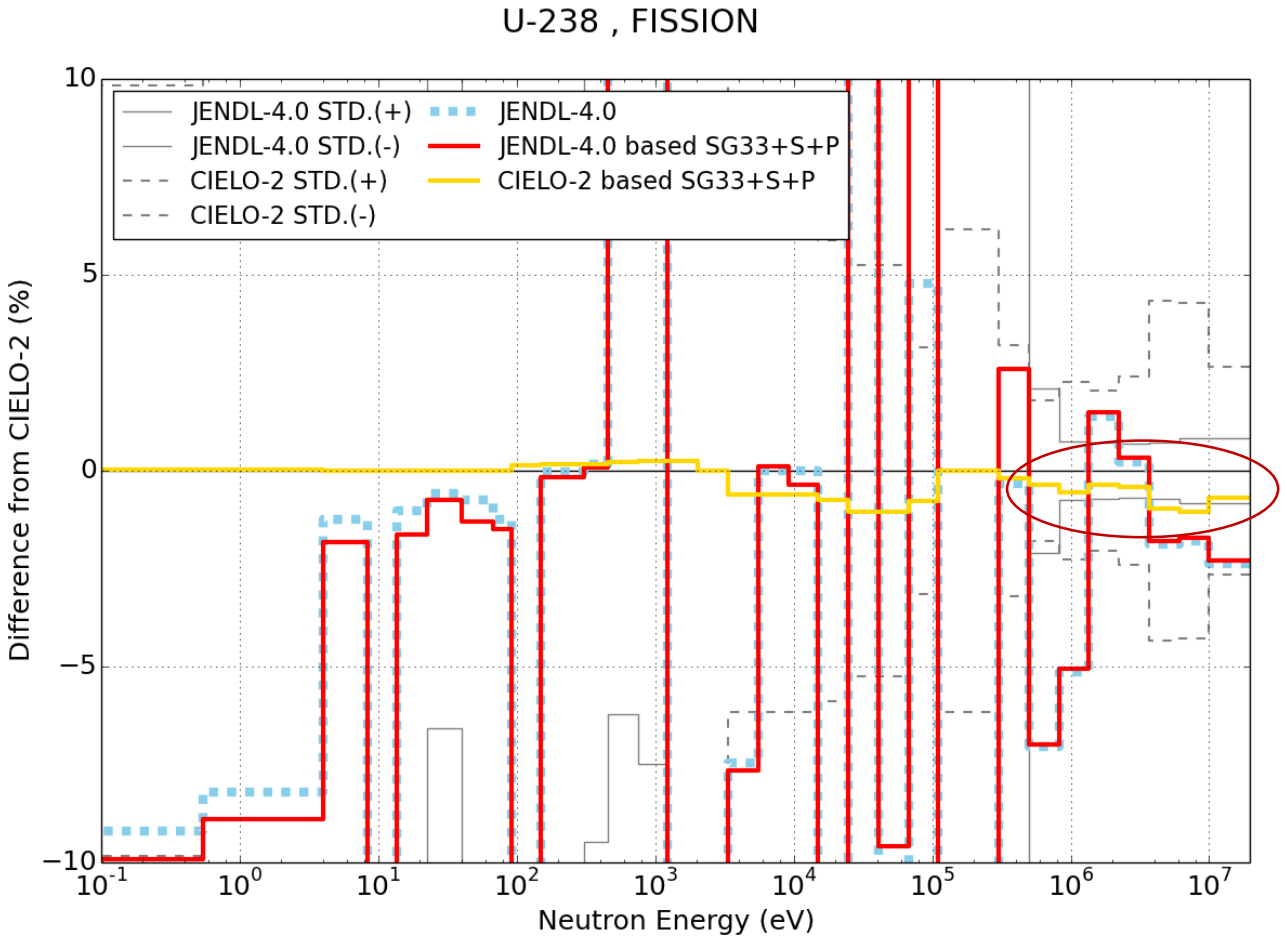
Fig. U-238 Capture vs. U-238 $\bar{\nu}$



- However, in U-238 of CIELO-2, there are very strong correlations between capture and nu-bar.
- When U-238 capture cross section is enlarged by adjustment, U-238 nu-bar becomes bigger by the positive correlations.
- This is a bad news for criticalities of SNEAK and PROTEUS.

- In CIELO-2, the inter-reaction correlations of U-238 seem to have big influence on the adjustment result.

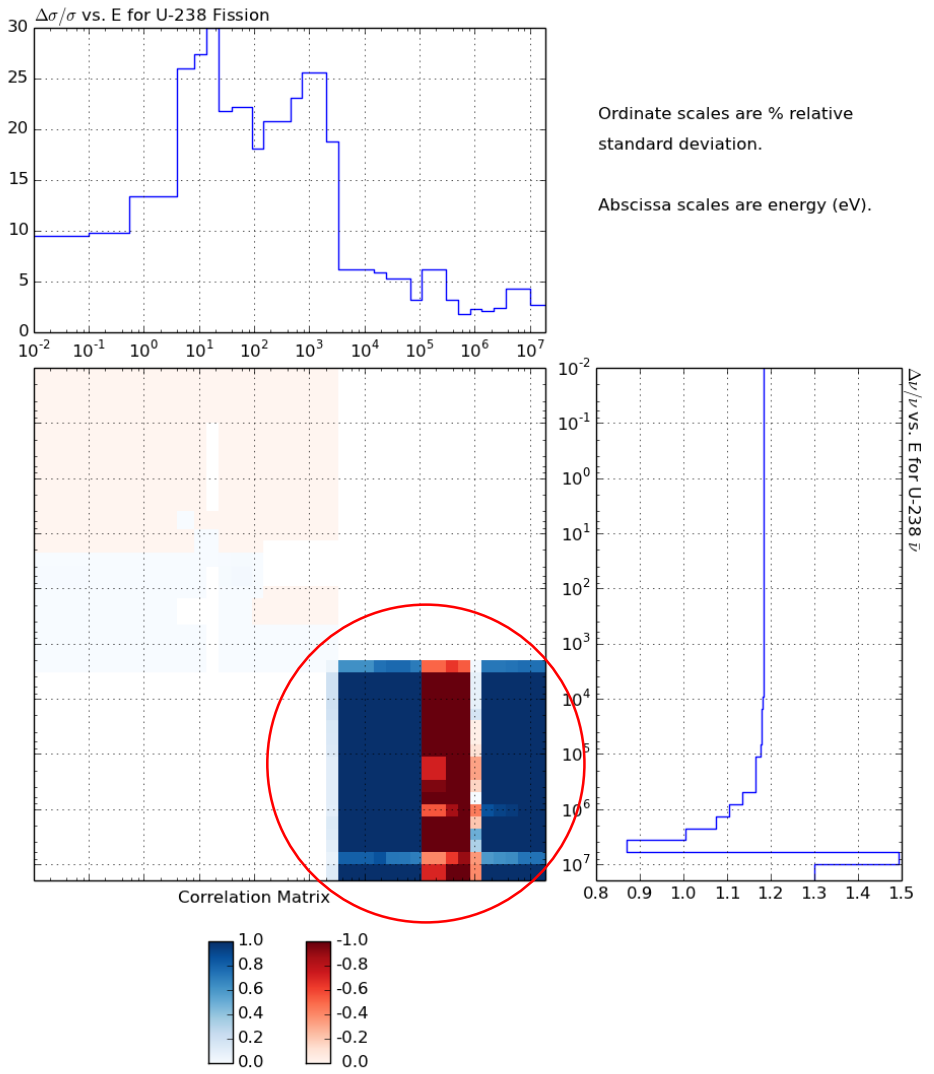
(2)-7 Adjustment of U-238 fission



- In CIELO-2, U-238 fission cross section was reduced by adjustment against the expectation from the C/E values of F28 RRRs.
- This adjustment may be caused by correlations.

(2)-8 Covariance of U-238 fission vs. capture

Fig. U-238 Fission vs. U-238 $\bar{\nu}$



- In U-238 of CIELO-2, there are very strong correlations between fission and nu-bar.
- When U-238 nu-bar is enlarged by adjustment, U-238 fission becomes smaller by the negative correlations.
- In CIELO-2, U-238 fission is also strongly correlated with capture, inelastic, elastic and (n,2n). It is difficult to determine the cause of the adjustment.

- In CIELO-2, the inter-reaction correlations of U-238 seem to have big influence on the adjustment result.

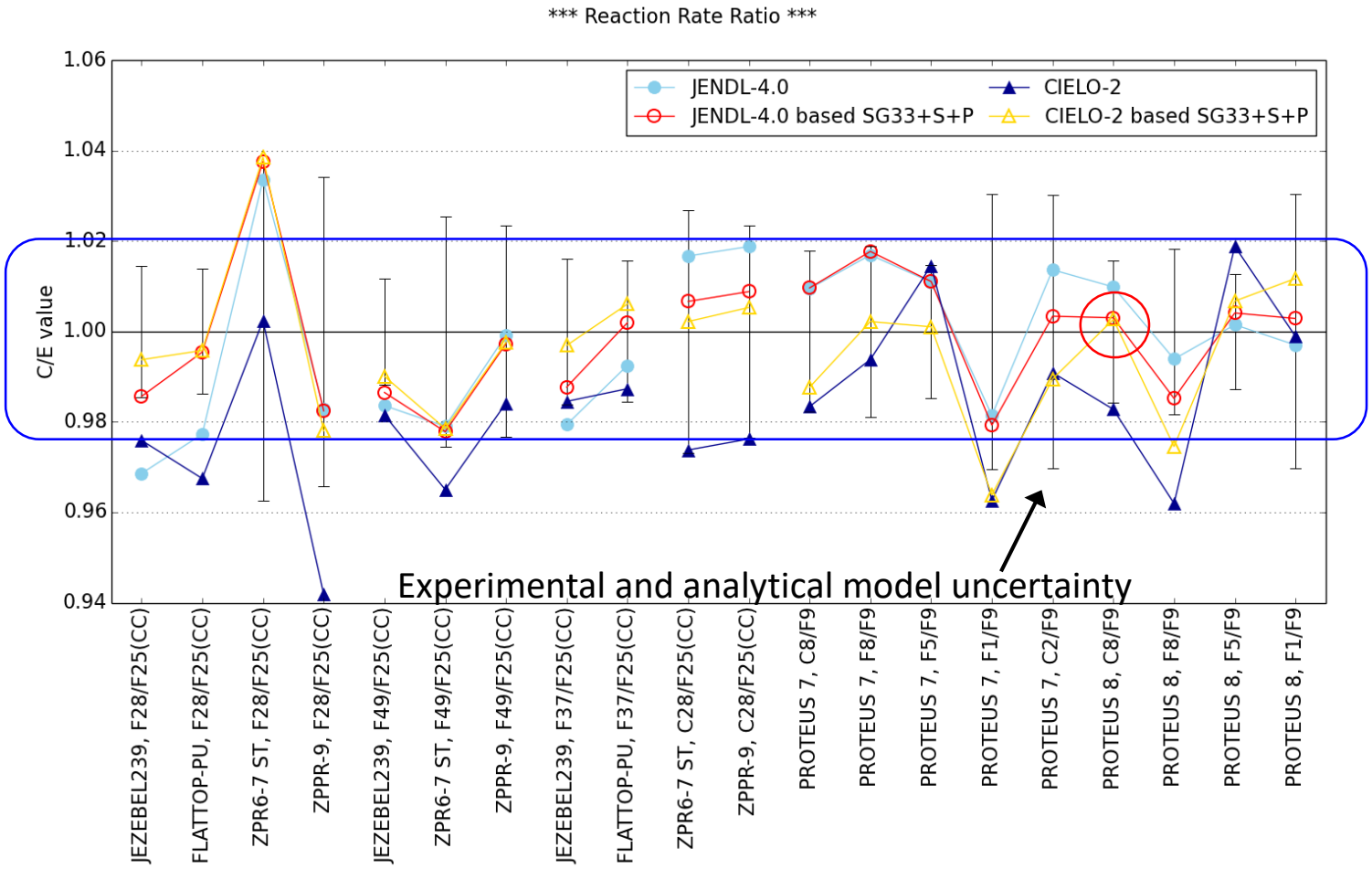
Summary (2)

- In the CIELO-2 based adjustment, the change of U-238 nu-bar is far exceeding 1-sigma uncertainty of CIELO-2.

- This is because there are very strong correlations in U-238 between almost all reactions, especially for the correlation between capture and nu-bar.

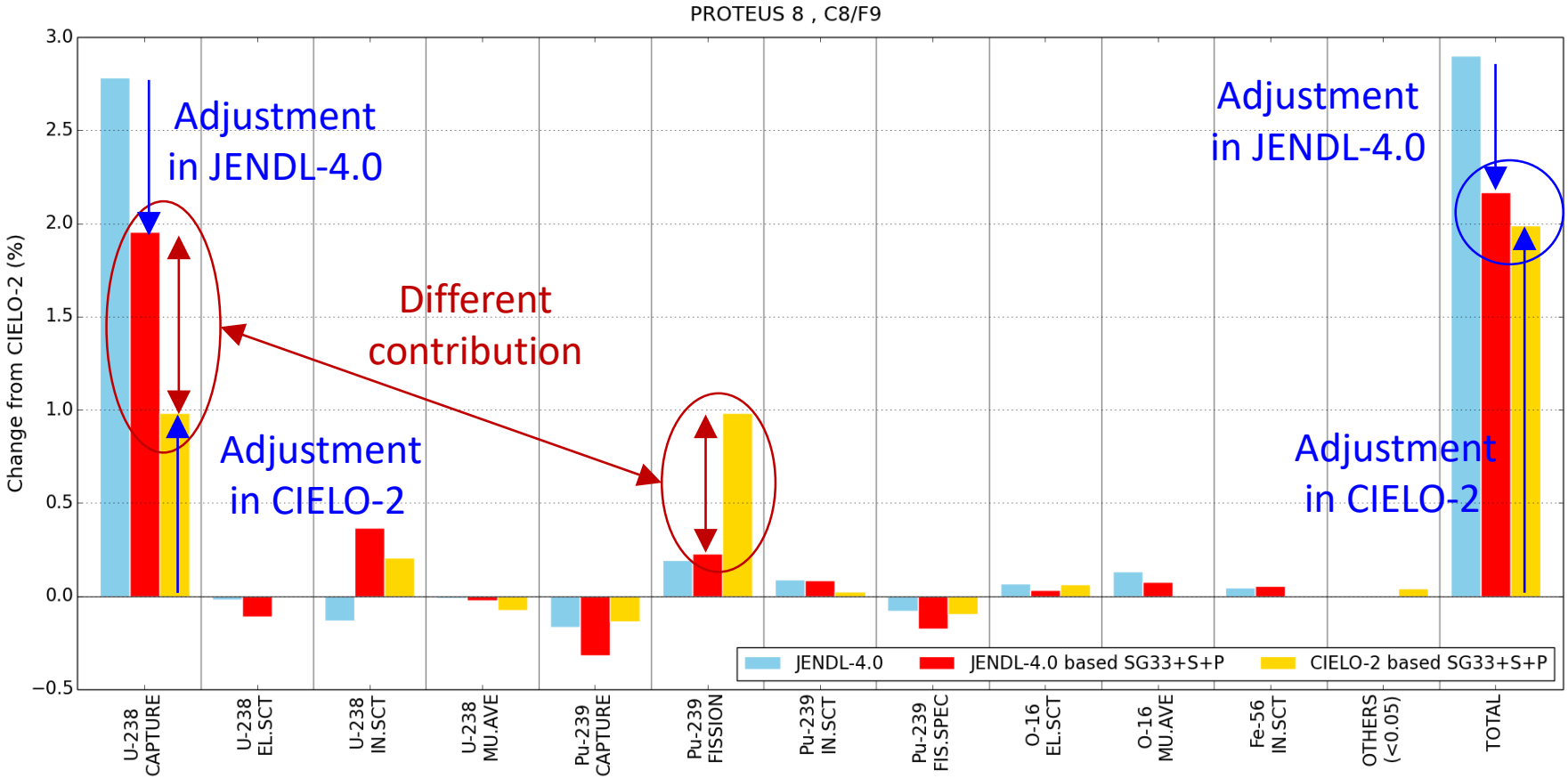
- C/E values of criticalities of SNEAK-7A, -7B, and PROTEUS 7 are not improved well.

(3)-1 RRR: C/E values



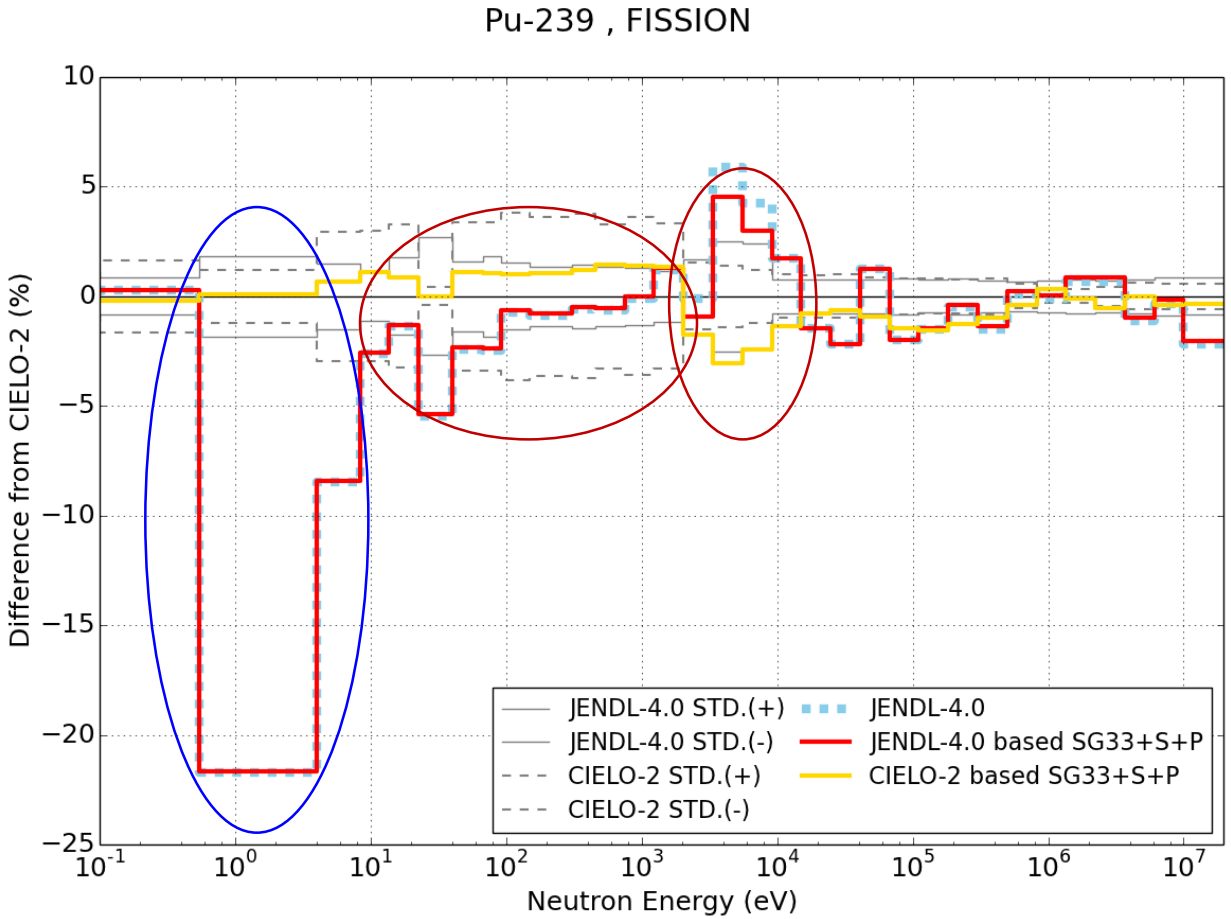
- In both JENDL-4.0 and CIELO-2, the posterior C/E values of reaction rate ratios (RRRs) are within the experimental and analytical model uncertainty.
- Let's focus on the C/E values of C28/F49 of PROTEUS 8, which are approximately unity both for JENDL-4.0 and CIELO-2.

(3)-2 Contributions to PROTEUS 8 C28/F49



- The posterior C/E value of PROTEUS 8 C28/F49 for JENDL-4.0 and CIELO-2 are almost the same, but the contributions are different.
- Even for RRRs, which are sensitive to only two reactions, we can find a typical compensation effect. (Perhaps, the compensation effect is inevitable when a criticality is used for adjustment.)

(3)-3 RRR: Adjustment of Pu-239 fission



- In two energy regions (10eV – 2keV and 2keV – 10keV) , the adjustment results are completely different and reversal.
- On the other hand, we can see a big difference between CIELO-2 and JENDL-4.0 in the lower energy region (around 1eV), which is far exceeding 1-sigma uncertainty.

(3)-4 RRR: Comparison of Pu-239 fission

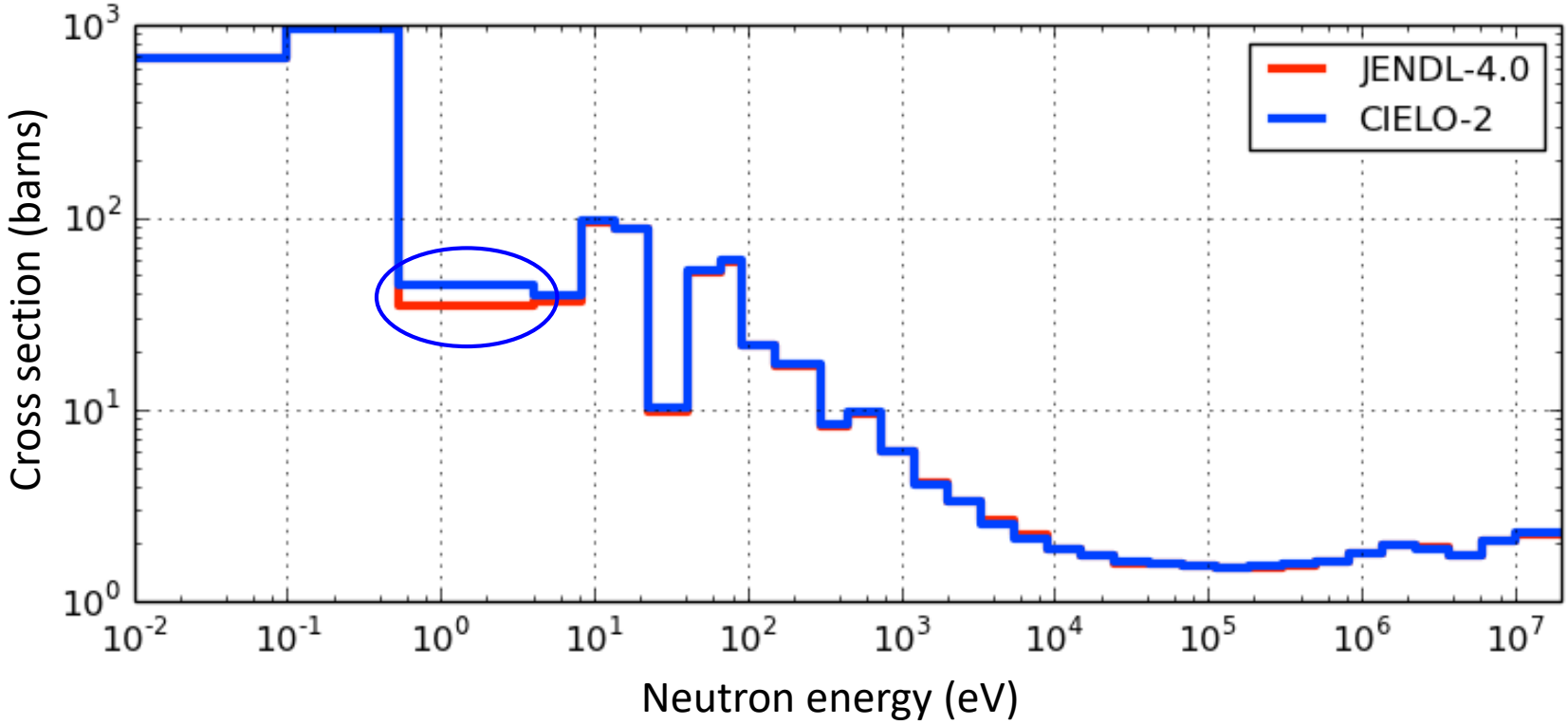


Fig. comparison of Pu-239 fission cross section

- The big difference between CIELO-2 and JENDL-4.0 is in the energy region above the giant resonance.

Summary (3)

- Even for the reaction rate ratios, such as C28/F49, which are sensitive only to two reactions, the contribution to C/E values are different. This is a typical compensation effect.

Appendix

- Details of HCLWR-PROTEUS (Core 7 and 8)
- Details of SNEAK (Core 7A and 7B)

HCLWR-PROTEUS

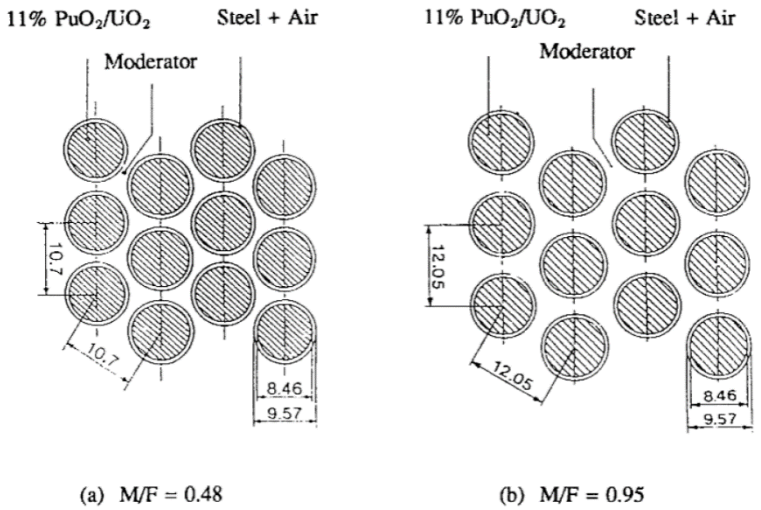
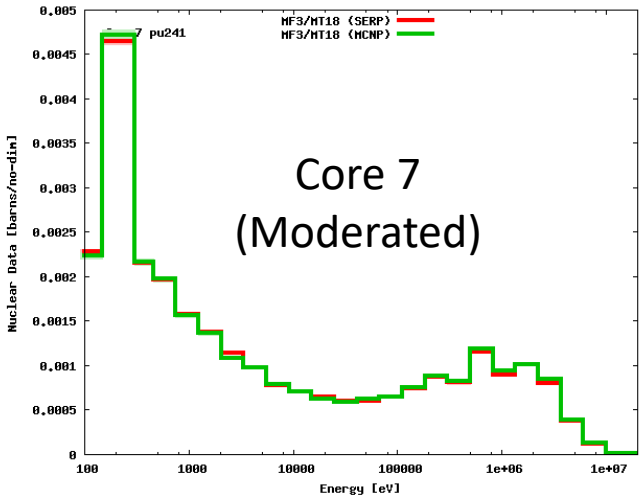


Fig.: Lattice description of the a) tight- and b) wide-pitch configuration*

Table: Nominal Pu vector of the reference date (01.01.1986)*

Isotope	Ratio
Pu-238	1%
Pu-239	64%
Pu-240	23%
Pu-241	8%
Pu-242	4%



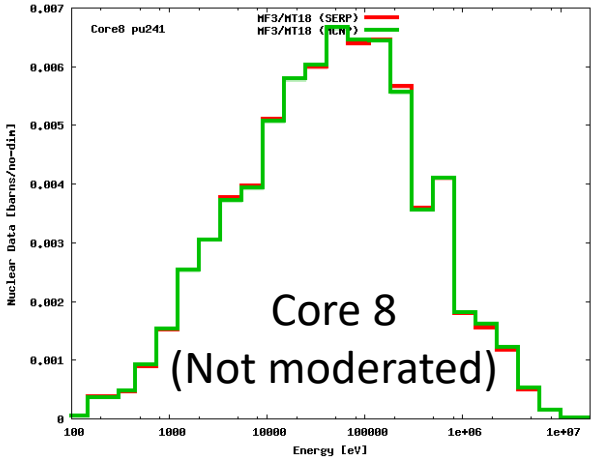


Fig.: Differential sensitivity of Pu-241 fission*

*: M. Hursin, et al., "Description of the Data provided to the SG39 with respect to the HCLWR experiments at Proteus," AN-41-15-05 V.1, PSI (2015)

Atomic Densities of PROTEUS Core 7 and 8

Table 2: Fuel Composition for Core 7 and Core 8

Isotope	Core7	Core8	Isotope	Core 7	Core 8
U-234	1.8496E-06	1.9480E-06	O-16	4.5841E-02	4.5841E-02
U-235	1.5996E-04	1.5996E-04	Fe-54	1.7857E-06	1.7857E-06
U-236	2.9158E-07	2.9158E-07	Fe-56	2.8239E-05	2.8239E-05
U-238	2.0492E-02	2.0492E-02	Fe-57	6.7734E-07	6.7734E-07
			Fe-58	8.6206E-08	8.6206E-08
Pu-238	2.3974E-05	2.3876E-05	Ca-40	9.3421E-06	9.3421E-06
Pu-239	1.5364E-03	1.5364E-03	Ca-42	6.2351E-08	6.2351E-08
Pu-240	5.5930E-04	5.5930E-04	Ca-43	1.3010E-08	1.3010E-08
Pu-241	1.7580E-04	1.7142E-04	Ca-44	2.0103E-07	2.0103E-07
Pu-242	8.4588E-05	8.4588E-05	Ca-46	3.8548E-10	3.8548E-10
Am-241	3.3298E-05	3.7678E-05	Ca-48	1.8021E-08	1.8021E-08

M. Hursin, et al., “Description of the Data provided to the SG39 with respect to the HCLWR experiments at Proteus,” AN-41-15-05 V.1, PSI (2015)

SNEAK-7A/7B

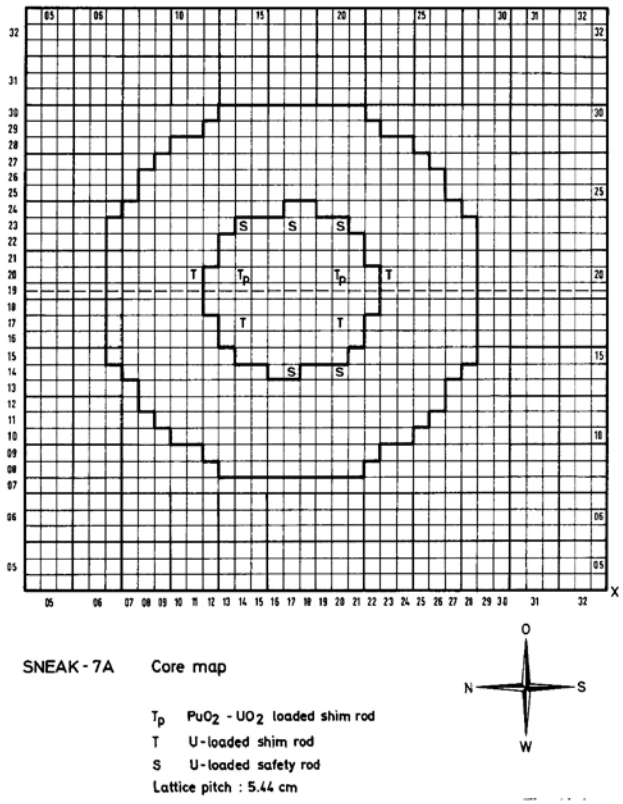


Fig.: SNEAK-7A Core Map*

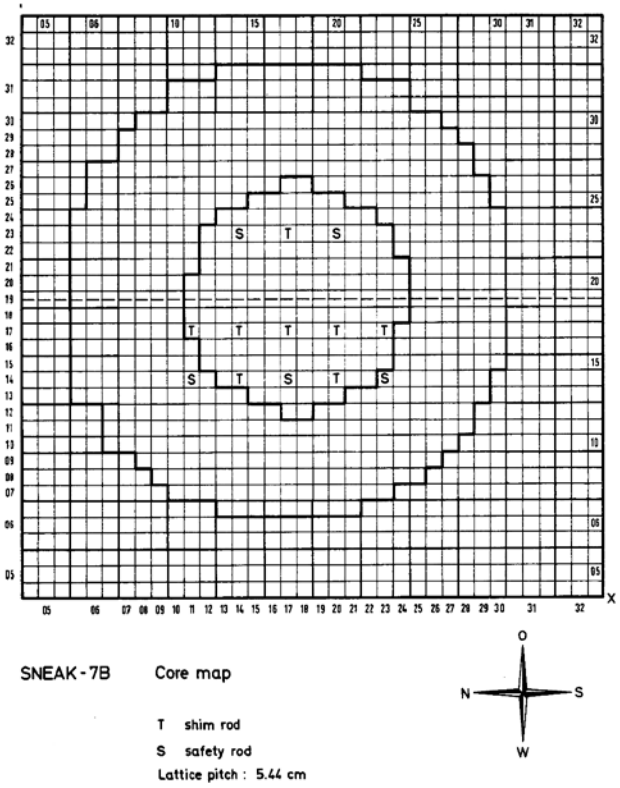


Fig.: SNEAK-7B Core Map*

*: E. Ivanov, et al., "SNEAK 7A and 7B Pu-fueled fast critical assemblies in the Karlsruhe fast critical facility," International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE), NEA/NSC/DOC(2006)1, March 2015 Edition

Table: Summary of Feature of SNEAK-7A and -7B*

Assembly	Year	Features	Core Components	Blanket
7A	1970/71	1-zone core	PuO2-UO2, graphite	Metallic depleted U
7B	1971		PuO2-Uo2, ^{nat}UO2	

Atomic Densities of SNEAK-7A/7B

Table 1.7. Atomic Densities for SNEAK-7A R-Z Model, 10^{24} cm^{-3} (Reference 1, p. 69).

Isotope	Inner Core	Outer Core	Blanket
Al	0.0000080	0.0011906 [(a)]	-
C	0.0260987	0.0255387	0.0000135
Cr	0.0022423	0.0022390	0.0011080
Fe	0.0079713	0.0079824	0.0039549
H	-	-	-
Mg	-	-	-
Mn	0.0001109	0.0001178	0.0000875
Mo	0.0000165	0.0000145	0.0000100
Nb	0.0000089	0.0000077	0.0000085
Ni	0.0011664	0.0011818	0.0009845
O	0.0218462	0.0211909	-
^{239}Pu	0.0026374	0.0023434	-
^{240}Pu	0.0002369	0.0002105	-
^{241}Pu	0.0000215	0.0000191	-
^{242}Pu	0.0000011	0.0000010	-
Si	0.0000933	0.0000932	0.0000453
^{235}U	0.0000586	0.0002958 [(b)]	0.0001624
^{238}U	0.0079604	0.0080456	0.0399401

(a) This value is 7.2% higher than the value calculated from stretched-platelet atom densities (Table 1.9).
(b) Note that this value is 5.9% higher than the value calculated using the described method for obtaining outer-core atom densities.

Table 1.8. Atomic Densities for SNEAK-7B R-Z Model, 10^{24} cm^{-3} (Reference 1, p. 71).

Isotope	Core	Blanket
Al	0.0012112	-
C	0.0000631	0.0000135
Cr	0.0027560	0.0011080
Fe	0.0098021	0.0039549
H	0.0000071	-
Mg	0.0000095	-
Mn	0.0000646 [(a)]	0.0000875
Mo	0.0000184	0.0000010 [(b)]
Nb	0.0000084	0.0000085
Ni	0.0014594	0.0009845
O	0.0331936	-
^{239}Pu	0.0018312	-
^{240}Pu	0.0001645	-
^{241}Pu	0.0000149	-
^{242}Pu	0.0000007	-
Si	0.0001174	0.0000453
^{235}U	0.0002663	0.0001624
^{238}U	0.0145794	0.0399401

(a) The calculated value for Mn using the method described in the previous paragraph is 94% larger than this value.
(b) This value was given as 0.0000100 for SNEAK 7A. All other blanket values are the same for both cores.

*: E. Ivanov, et al., “SNEAK 7A and 7B Pu-fueled fast critical assemblies in the Karlsruhe fast critical facility,” International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE), NEA/NSC/DOC(2006)1, March 2015 Edition

C/E values of SNEAK-7A/7B

Table: C/E and experimental uncertainty on keff for SNEAK-7A and 7B

	Calculation	Experiment	C/E
SNEAK-7A KEFF	1.0064$_{97}$	1.0010 +- 0.0029	1.0054$_{9}$ +- 0.0029
SNEAK-7B KEFF	1.0058$_{63}$	1.0016 +- 0.0035	1.0042$_{6}$ +- 0.0035

I. Kodeli, "Sensitivities profiles: Flattop-Pu, SNEAK-7A, SNEAK-7B, ASPIS-FE88," WPEC/SG39 website, https://www.oecd-nea.org/science/wpec/sg39/

- Conversion of C/E value (ENDF/B-VII.1 → JENDL-4.0)
  - Core 7: +0.452% (C/E = 1.0054$_{9}$ → 1.0100$_{1}$)
  - Core 8: +0.503% (C/E = 1.0042$_{6}$ → 1.0092$_{9}$)