WPEC SG39 Meeting, May 16-17, 2017
OECD/NEA, Paris, France

JENDL-4.0 Based Cross-section Adjustment by Adding New Experiments on the Basis of the SG33 Benchmark (Revised)

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Background

- In the last SG39 meeting, JAEA presented 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, PSI provided the updated sensitivity coefficients and new reaction data (spectral indices) of PROTEUS to SG39 members

The cross section adjustment results are revised with the updated PROTEUS data

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 (Updated)

- PROTEUS data provided by PSI (Paul Scherrer Institute)
  - 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

*: added after the last SG39 meeting

- SNEAK data provided by JSI (Jozef Stefan Institute)
  - 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 JENDL-4.0 by using sensitivity coefficients:

$$C_{JENDL-4.0} = C_x \times \left(1 + S_x \frac{\sigma_{JENDL-4.0} - \sigma_x}{\sigma_x} \right)$$

- 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 <u>are tentatively set to 0.5</u>
      - 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)	Library Effect	C/E (JENDL-4.0)	Rejected
Core 7	Kinf	1.008±0.006	+0.36%	1.0116	
Core 8	Kinf	0.996±0.004	+0.26%	0.9986	
Core 7/8	Void reactivity	0.78±0.11	-8.08%	0.7169	✓
Core 7	C28/F49	1.012±0.018	-0.20%	1.0100	
	F28/F49	1.006±0.019	+1.09%	1.0170	
	F25/F49	1.015±0.015	-0.34%	1.0116	
	F41/F49	0.988±0.030	-0.63%	0.9818	
	C42/F49	1.024±0.031	-0.88%	1.0150	
Core 8	C28/F49	1.021±0.016	-0.94%	1.0114	
	F28/F49	0.984±0.018	+1.17%	0.9955	
	F25/F49	1.025±0.013	-2.18%	1.0026	
	F41/F49	1.022±0.031	-2.35%	0.9980	
	C42/F49	1.229±0.037	-4.87%	1.1691	✓

*: 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)

Updated Sensitivity Coefficients

Adjusted nuclides and reactions		SNEAK 7A & 7B	PROTEUS 7 & 8	
			Previous	Present
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	●		🔴

Adjusted nuclides and reactions		SNEAK 7A & 7B	PROTEUS 7 & 8	
			Previous	Present
B-10	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 of fission spectrum and mu-average are added.
- For SNEAK, sensitivity coefficients of C-12, Cr-52 and Ni-58 are missing but they should be not important.

Adjustment Cases

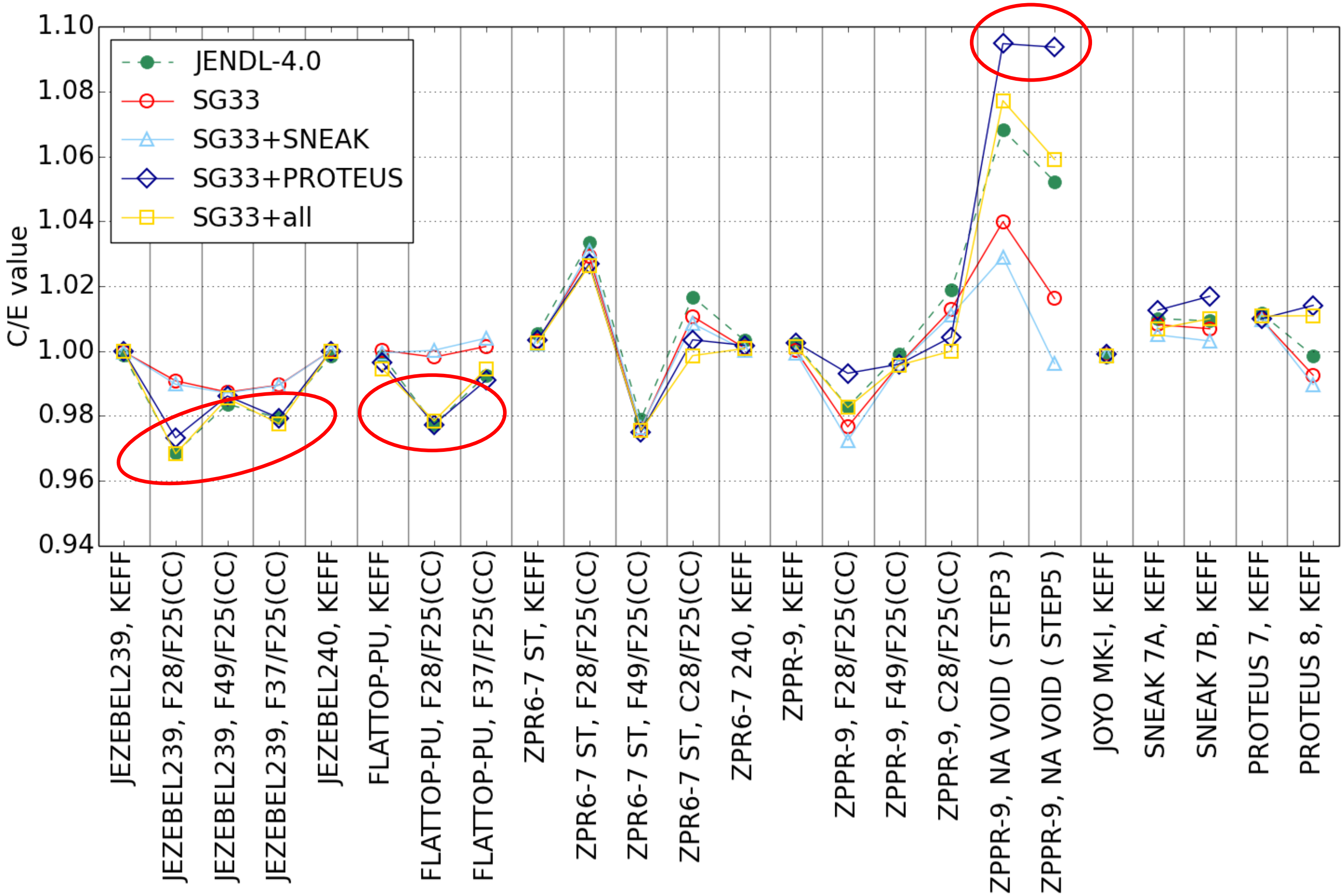
- Case1: “SG33”
  - The original integral experiment dataset of SG33 benchmark (20 data)

- Case2: “SG33 + SNEAK”
  - 2 KEFF(k_{eff})s of SNEAK are added to the SG33 dataset (22 data)

- Case3: “SG33 + PROTEUS”
  - 2 KINF(k_{∞})s and 9 RRR(reaction rate ratio)s of PROTEUS are added to the SG33 dataset (31 data)

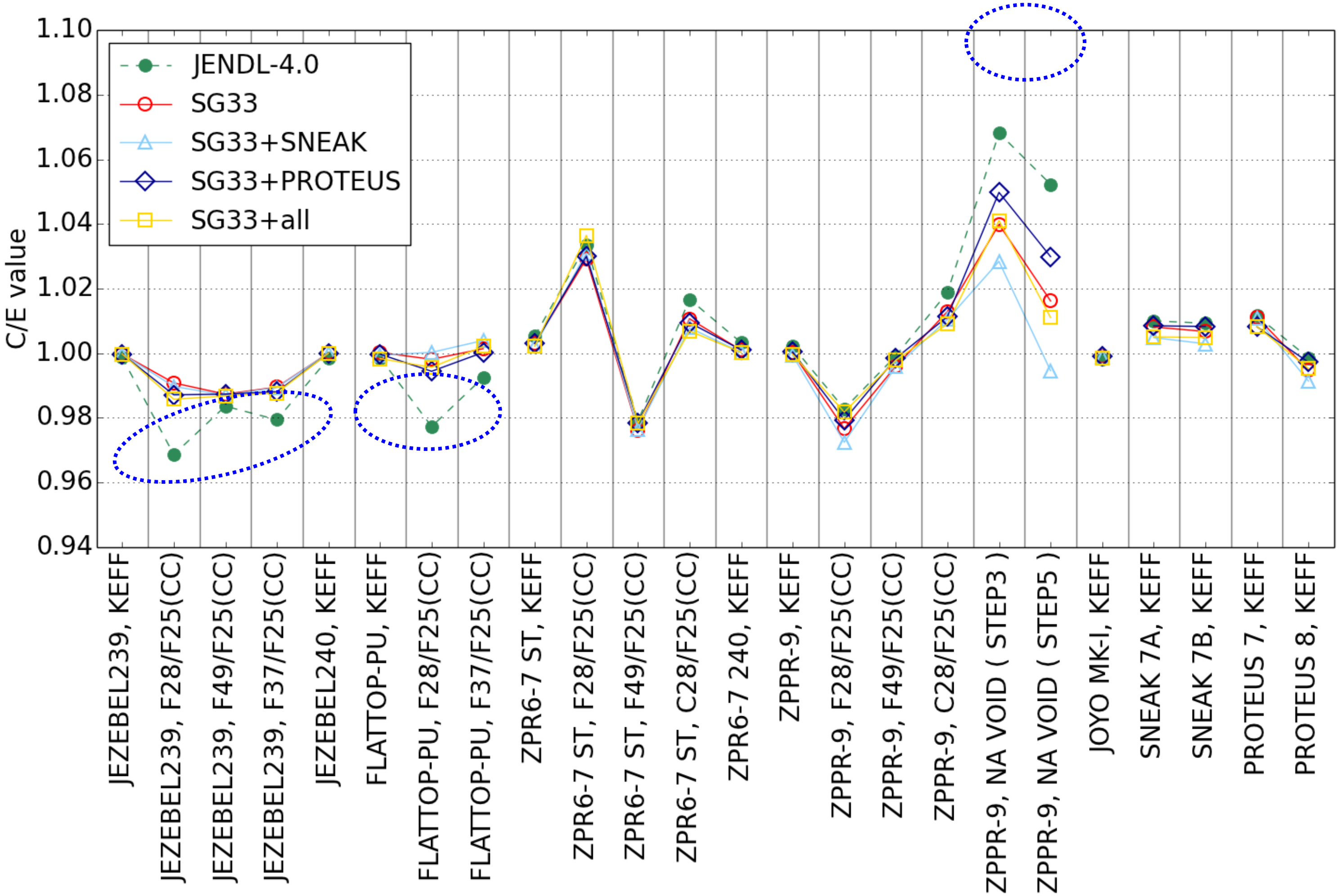
- Case4: “SG33 + all”
  - Both “SNEAK” and “PROTEUS” data are added to the SG33 dataset (33 data)

The previous result: C/E Values



- C/E values of JEZEBEL and FLATTP-PU are not improved when adding PROTEUS
- Addition of PROTEUS worsens the C/E values of ZPPR-9 sodium void worth

New result: C/E values



- C/E values of JEZEBEL and FLATTP-PU are improved when adding PROTEUS
- Addition of PROTEUS does not worsen the C/E values of ZPPR-9 sodium void worth

The previous result: Contributions

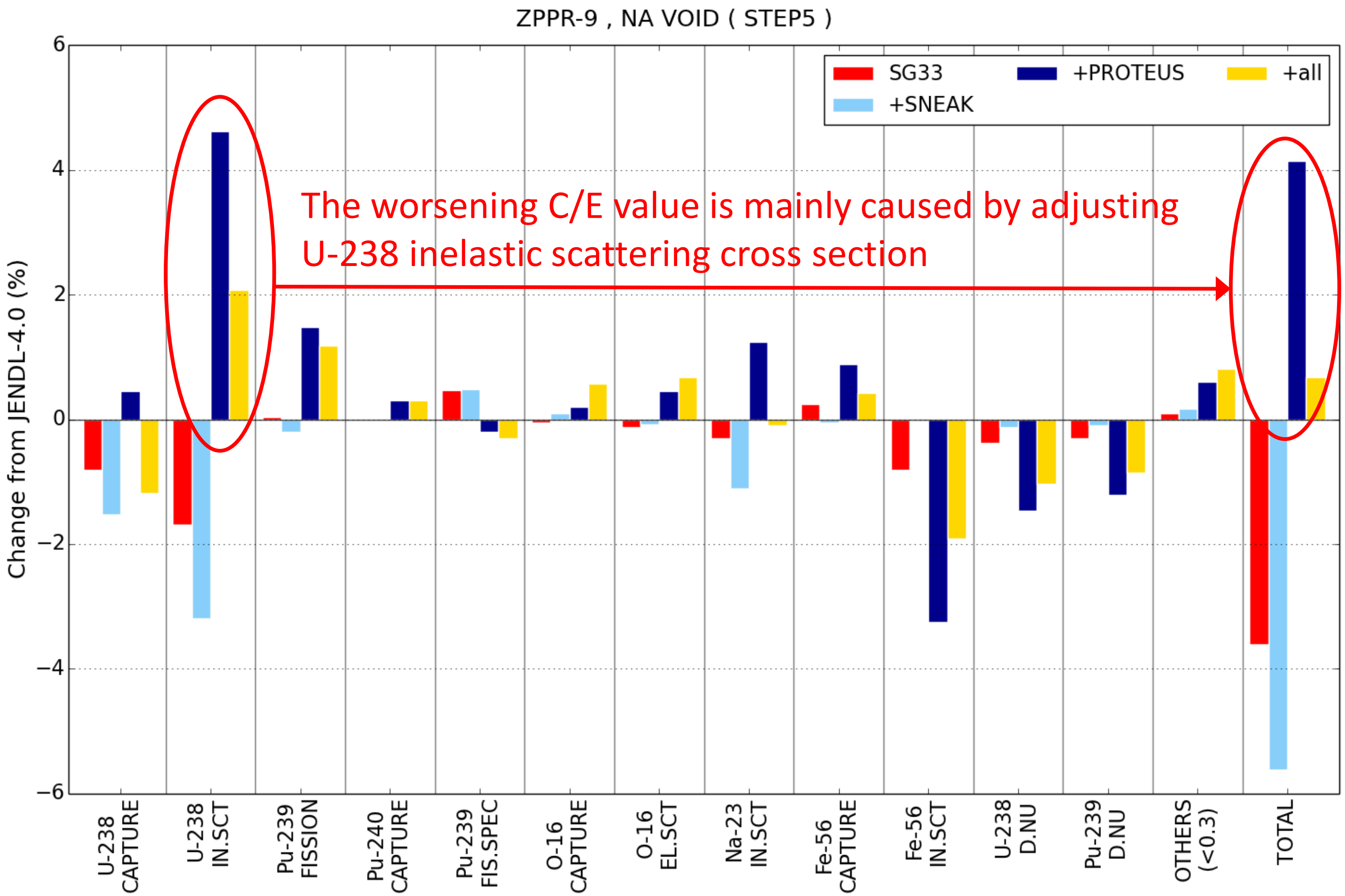


Fig. Reaction-wise contributions for C/E value of ZPPR-9 sodium void reactivity (Step5)

New results: Contributions

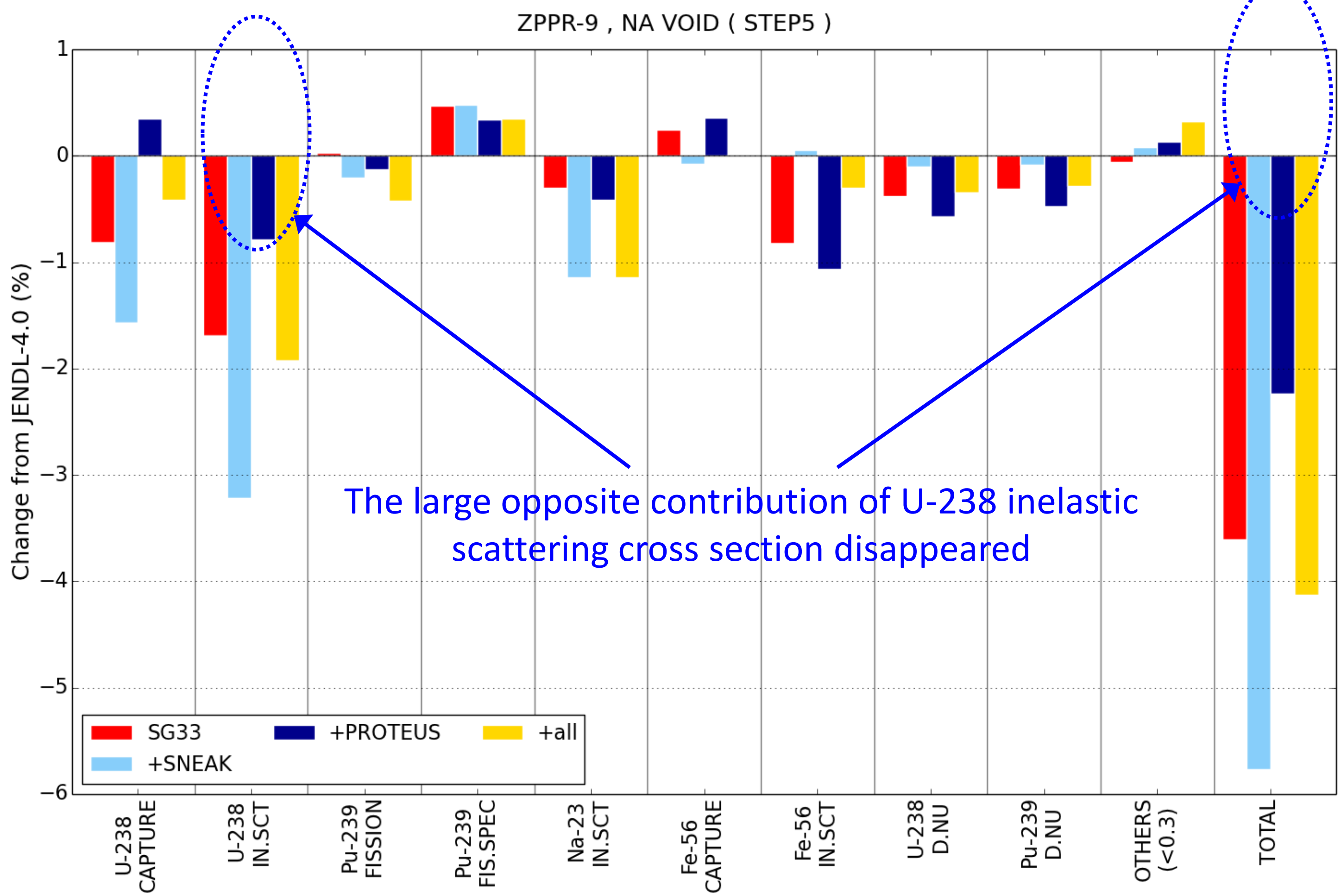
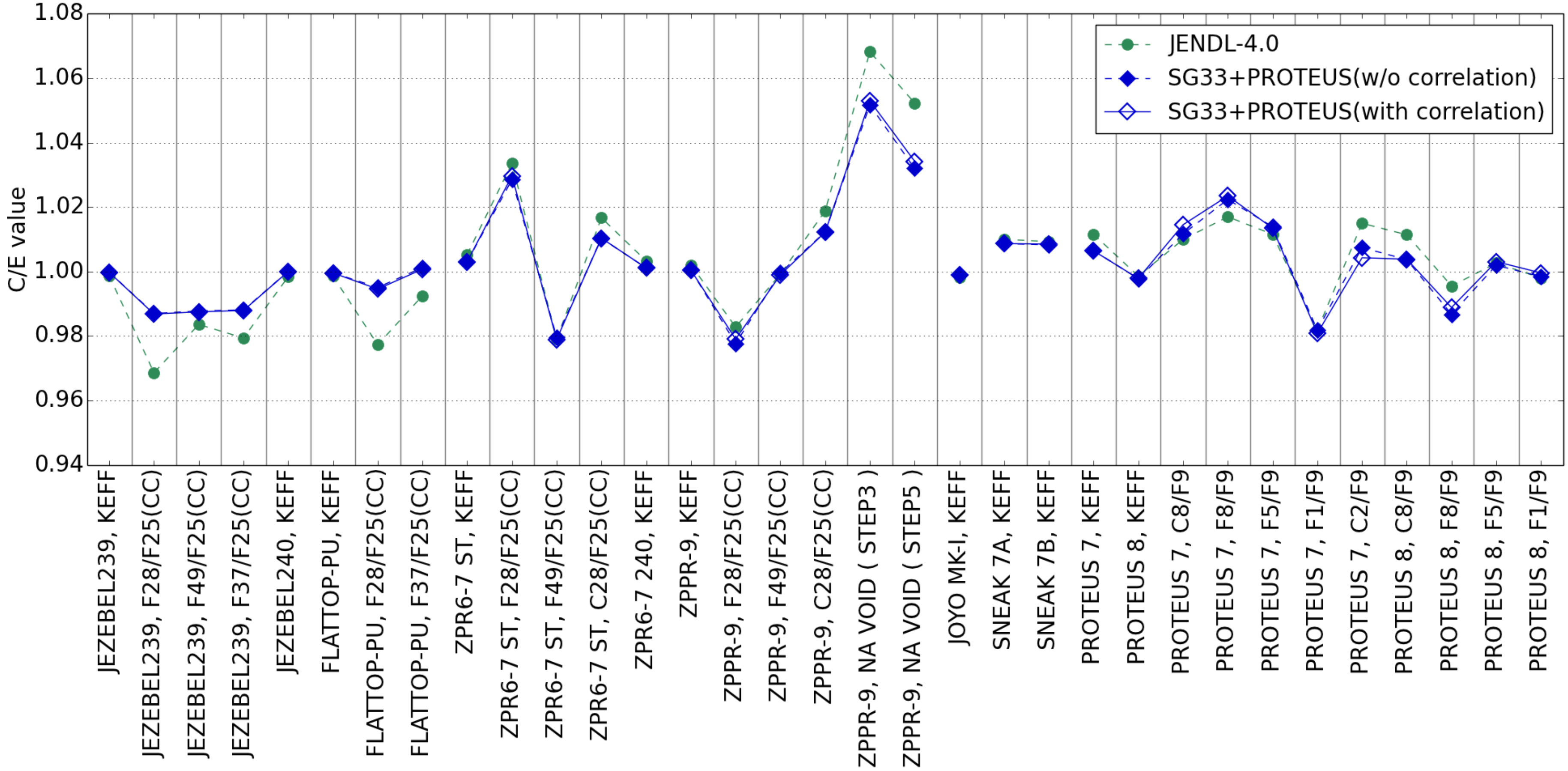


Fig. Reaction-wise contributions for C/E value of ZPPR-9 sodium void reactivity (Step5)

- Addition of sensitivity coefficients of fission spectrum solved the problem of the compensation effect among U-238 inelastic and fission spectrums

Effect of Correlation of PROTEUS Spectral Indices



- As mentioned before, correlation factors among spectral indices of PROTEUS are tentatively set to 0.5
- Fortunately, these correlation factors hardly affect the adjustment results for this case

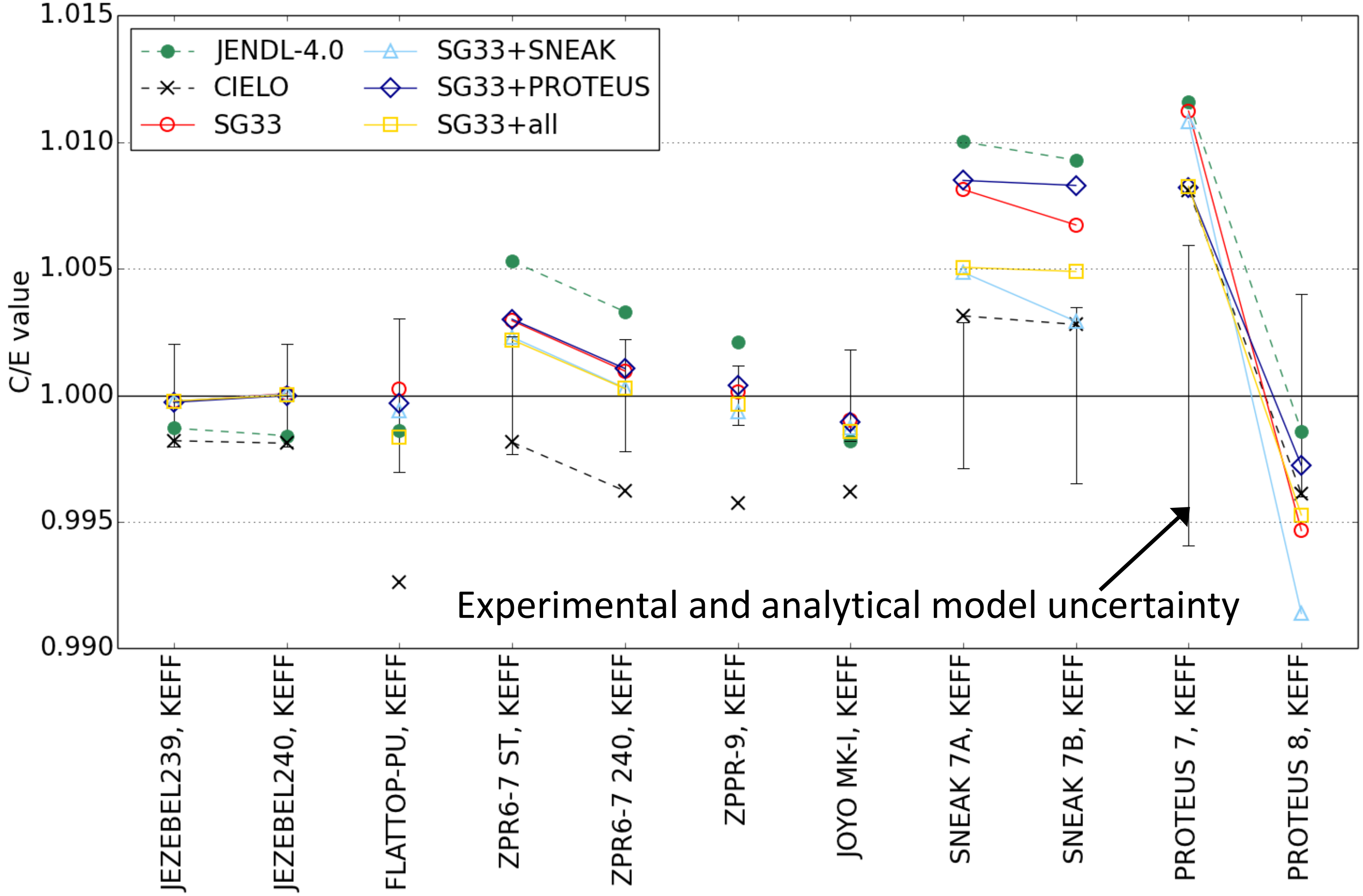
Detailed Versions of CIELO

All the CIELO files were downloaded from

https://www-nds.iaea.org/CIELO/

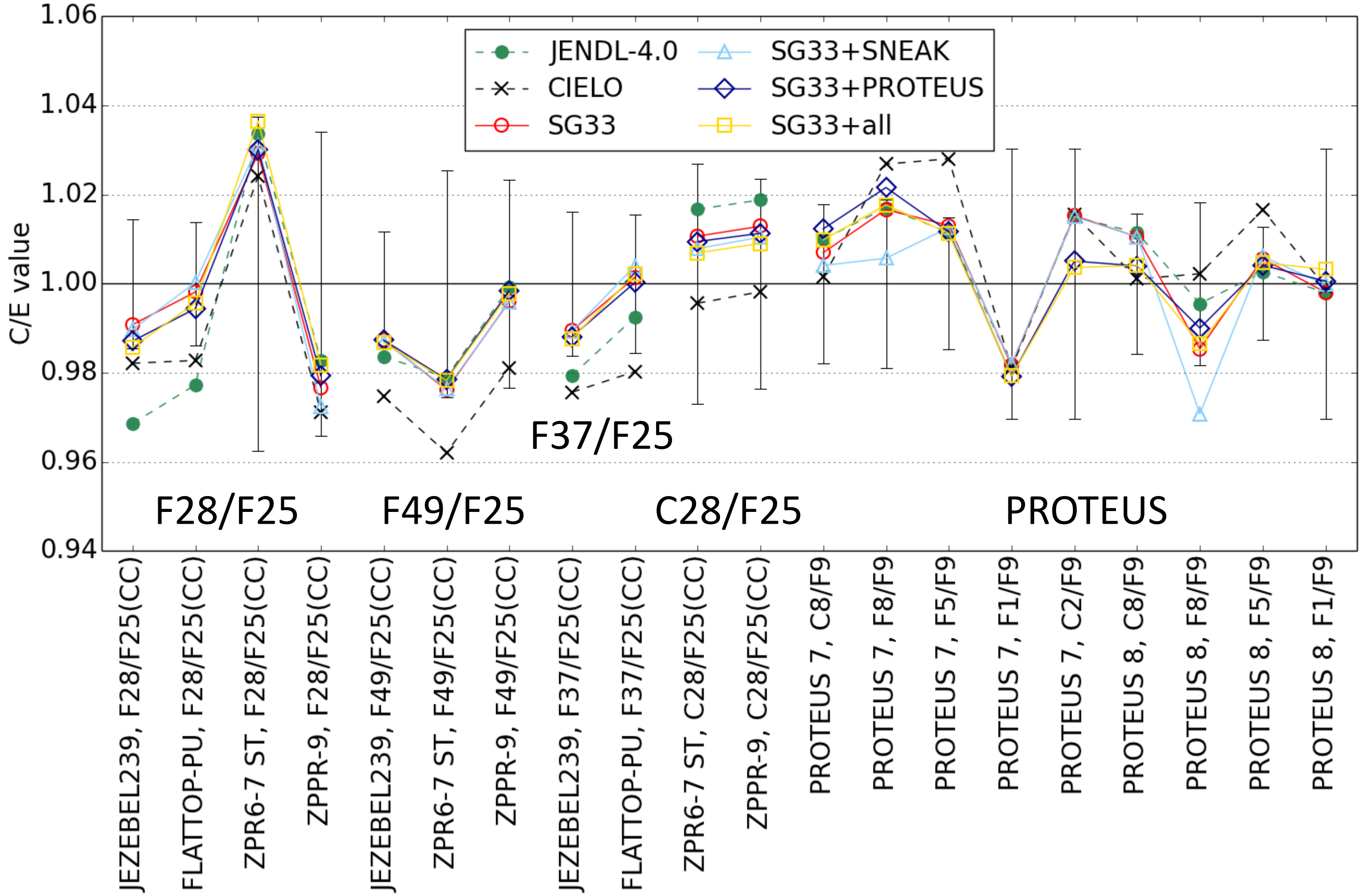
- IAEA-CIELO as of 15 Feb. 2017
  - U-235 Version: u235_CIELO20170215 compressed ENDF file (internal IAEA designation u235ib36o28t6DNcnu5ef0STs)
  - U-238 Version:u238_CIELO20170215 compressed ENDF file (internal IAEA designation u238ib54lrlFsfaST4d)
- LANL Pu-239 (17-22) Feb. 2017
  - Pu-239 Version: pu239e80b4_5_corDN (as submitted by D. Neudecker on 22 February) compressed ENDF file
- IAEA CIELO iron files (in collaboration with BNL-NNDC)
  - Fe-56 (26FEB) Version: fe56ib20w compressed ENDF file and compressed ACE file
- Available Materials
  - O-16 Version: o16e80b1, ENDF/B-VIII beta1 file (filename: n_008_O_016_b0.endf)

C/E Values: Criticality



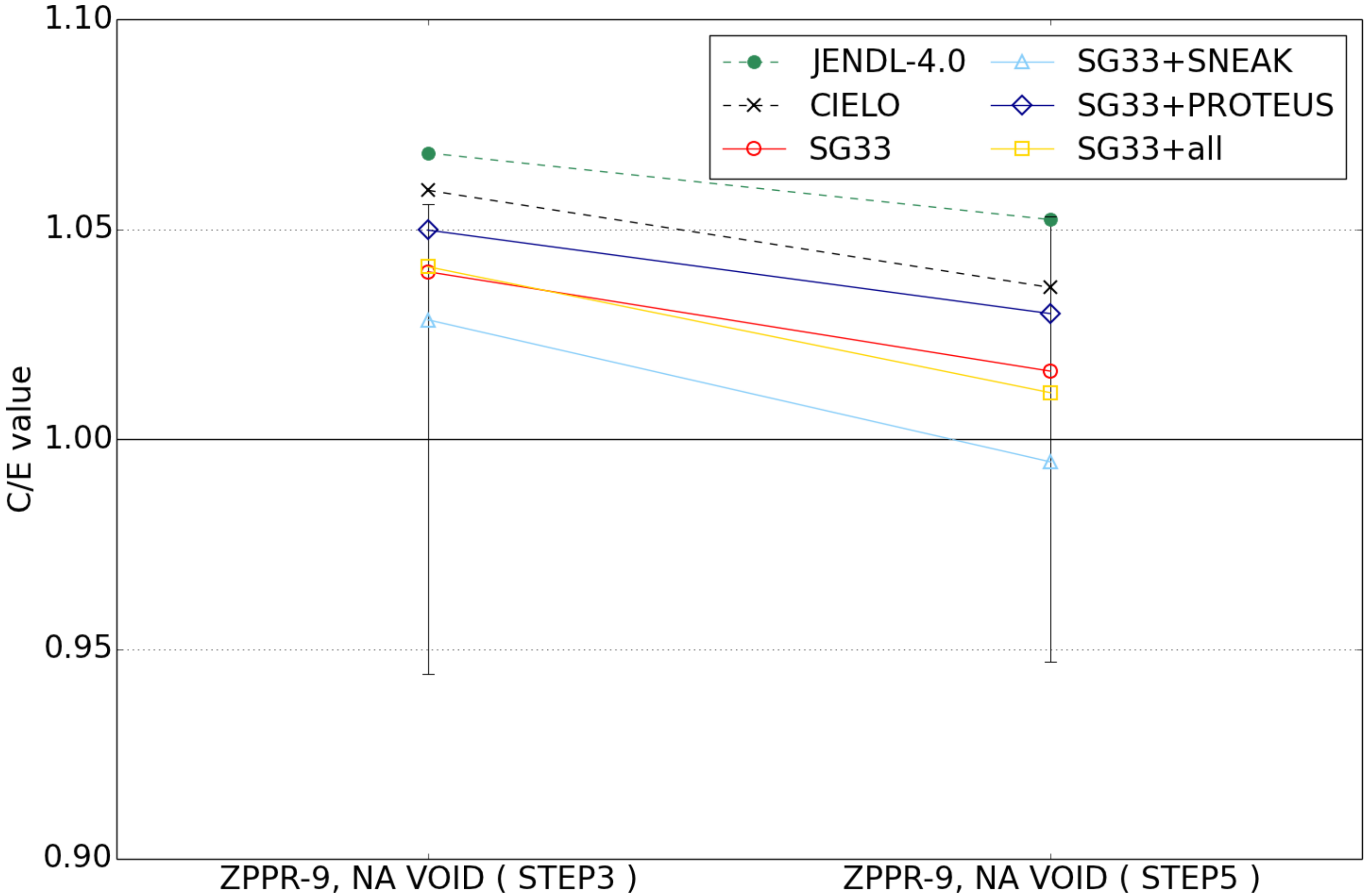
- Both SNEAK and PROTEUS seem to be consistent with the original SG33 benchmark. (= They do not affect C/E values of the SG39 dataset.)
- C/E values of PROTEUS are not improved well(?).

C/E Values: Reaction Rate Ratios



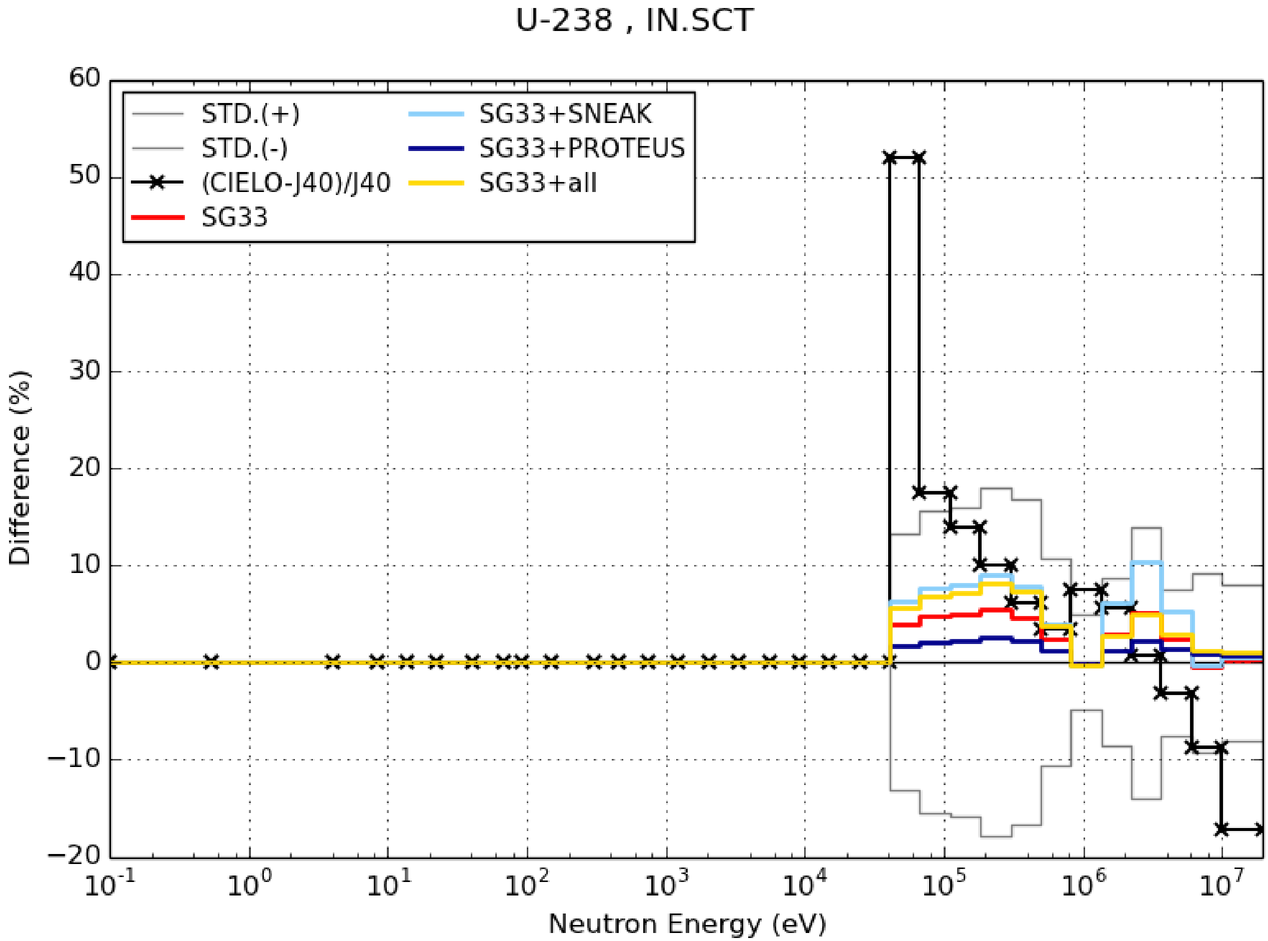
- All cases of SG33, SG33+SNEAK, SG33+PROTEUS, and SG33+all improve C/E values of reaction rate ratios (spectral indices).

C/E Values: Void Reactivity Worth



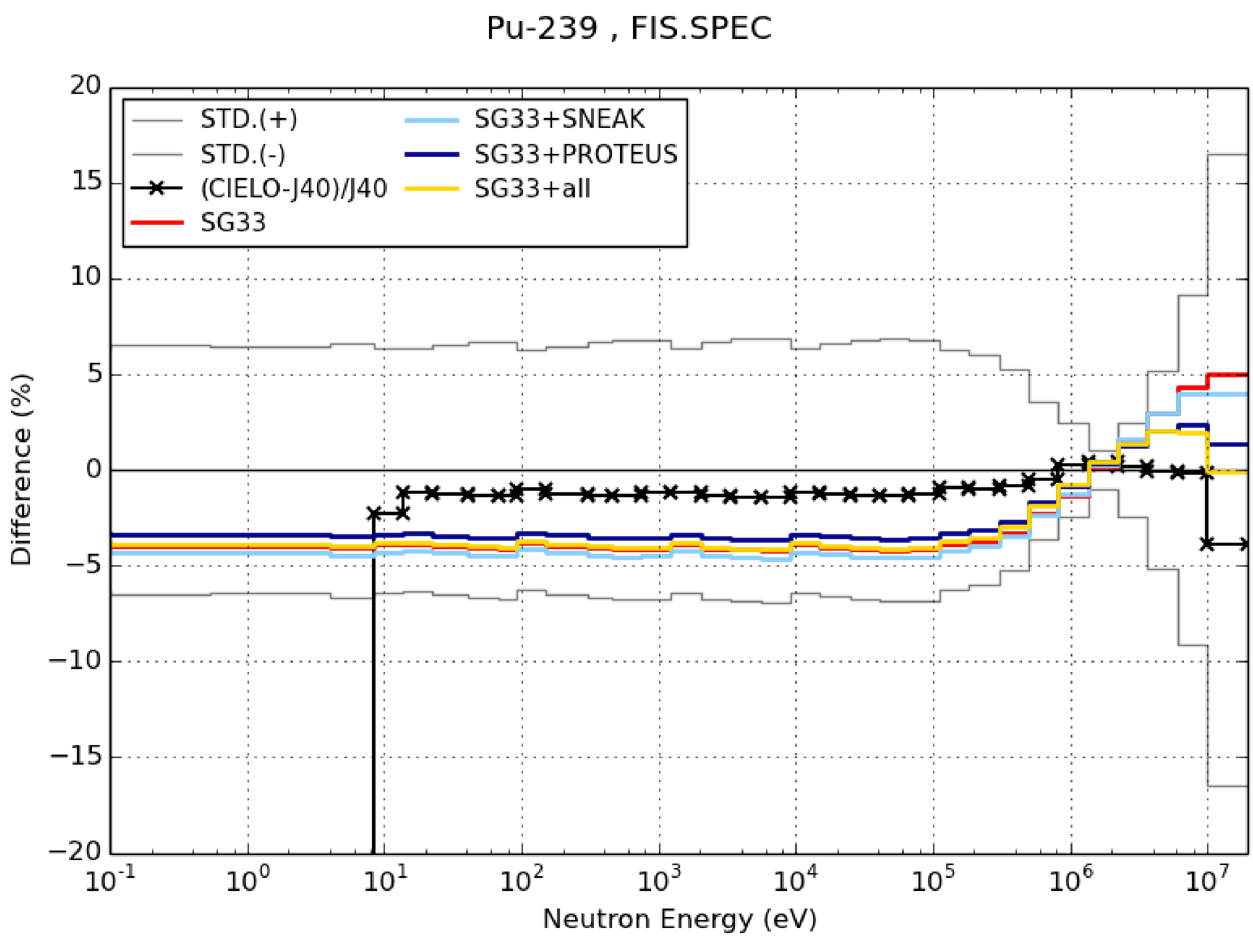
- All cases of SG33, SG33+SNEAK, SG33+PROTEUS, and SG33+all improve C/E values of ZPPR-9 sodium void reactivity.

U-238 inelastic scattering cross sections



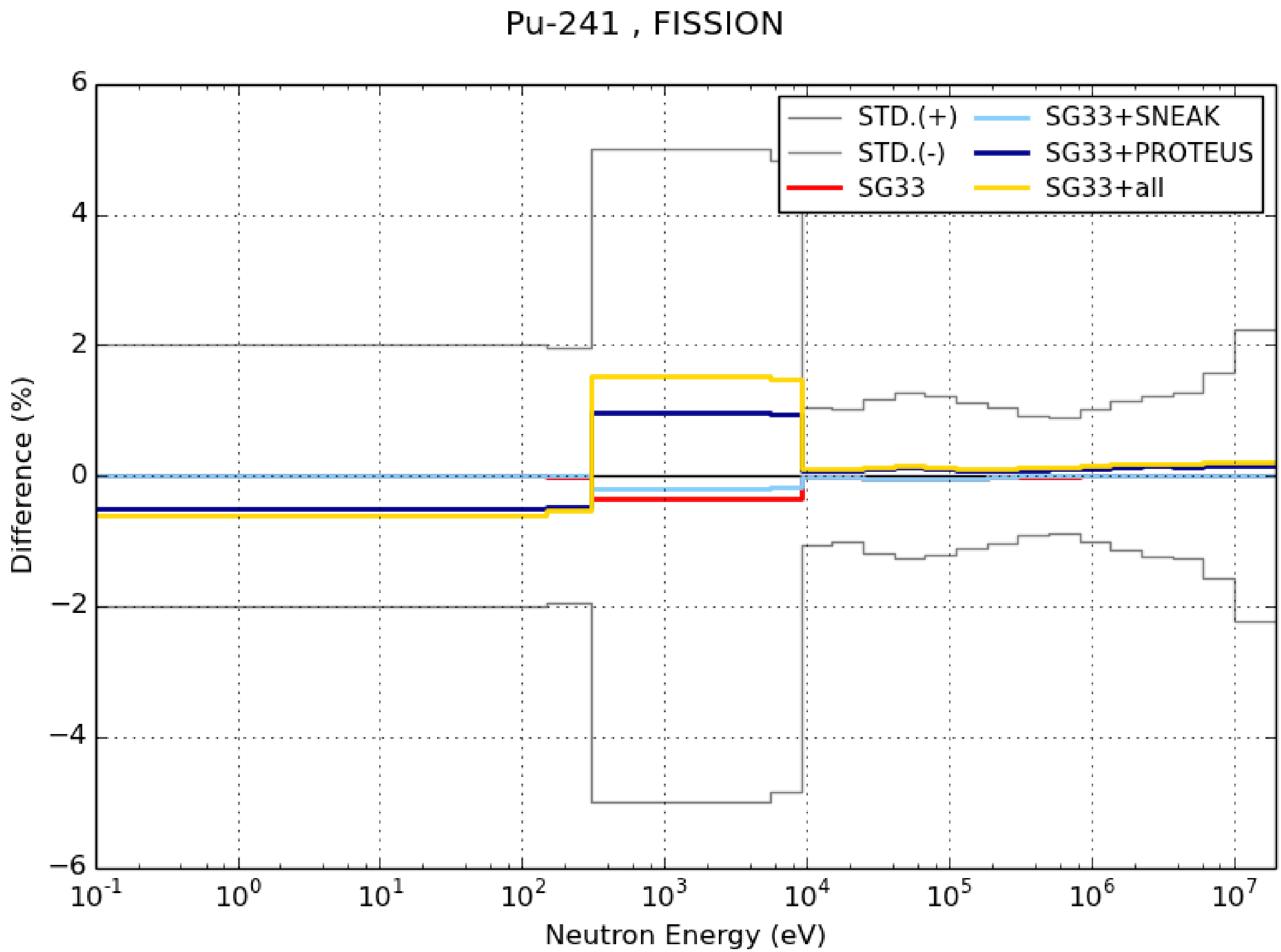
- SNEAK and PROTEUS increase U-238 inelastic scattering cross section.
- Even though U-238 inelastic scattering cross section may have a typical compensation effect with fission spectrums, could we say that these results support the evaluation of CIELO?

Pu-239 fission spectrum



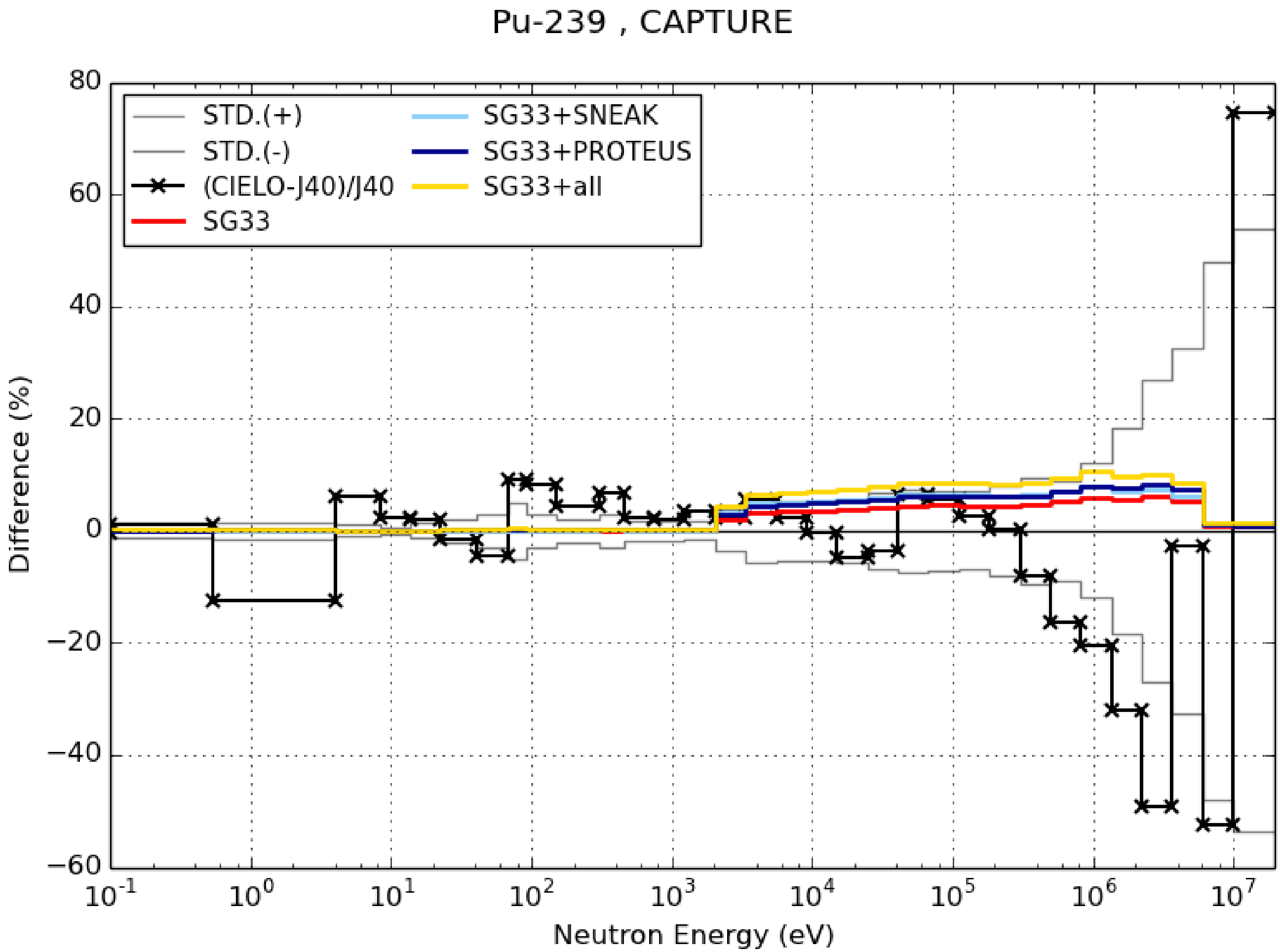
- Both PROTEUS and SNEAK have a tendency to make the neutron spectrum harder.
- According to the adjustment result of U-238 inelastic cross section, they require softer neutron spectrum. (Is it a compensation effect?)

Pu-241 fission cross sections



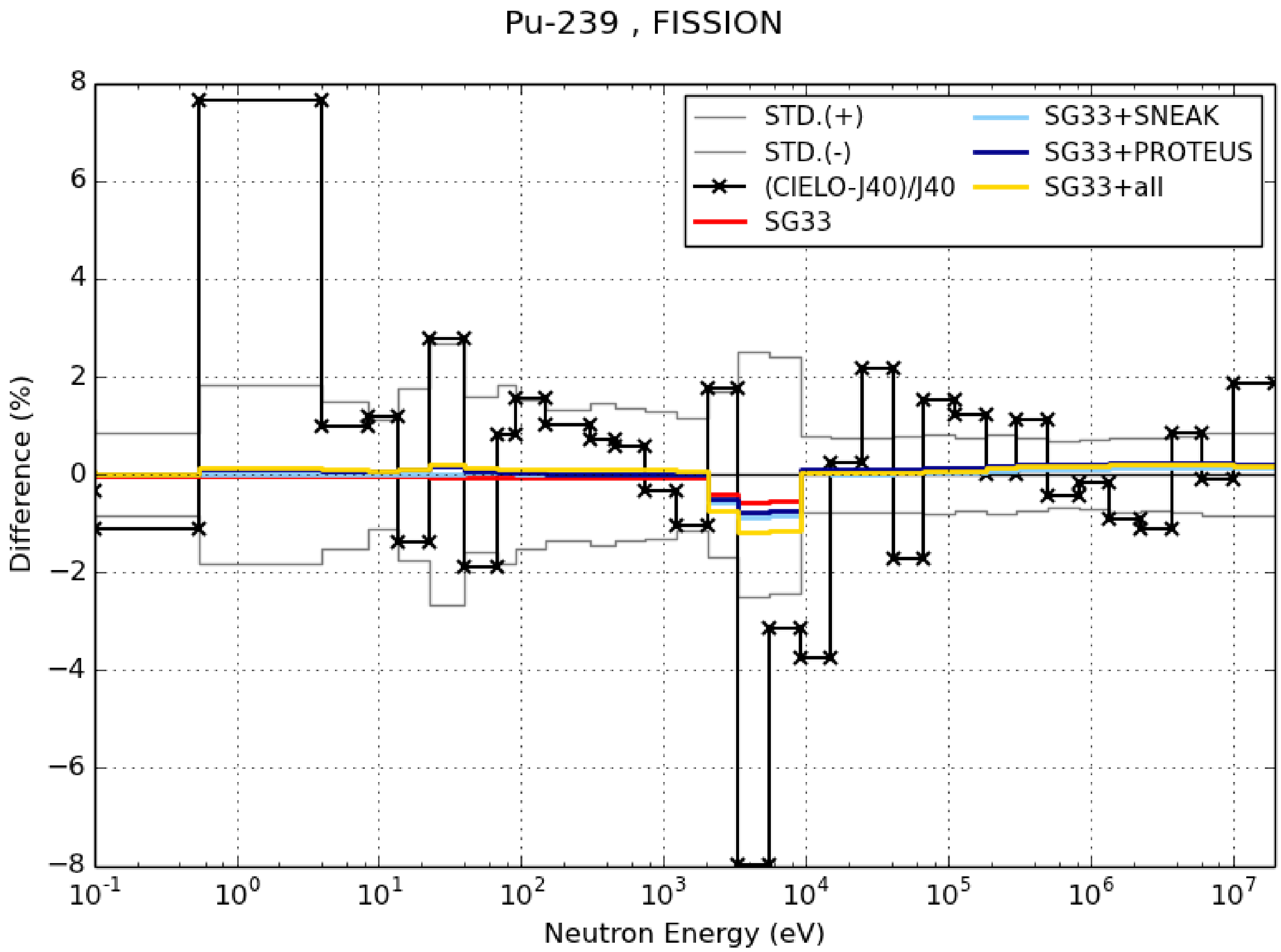
- Addition of PROTEUS increases Pu-241 fission cross section in above keV ranges.
- PROTEUS also includes the information in lower energy ranges.

Pu-239 capture cross sections



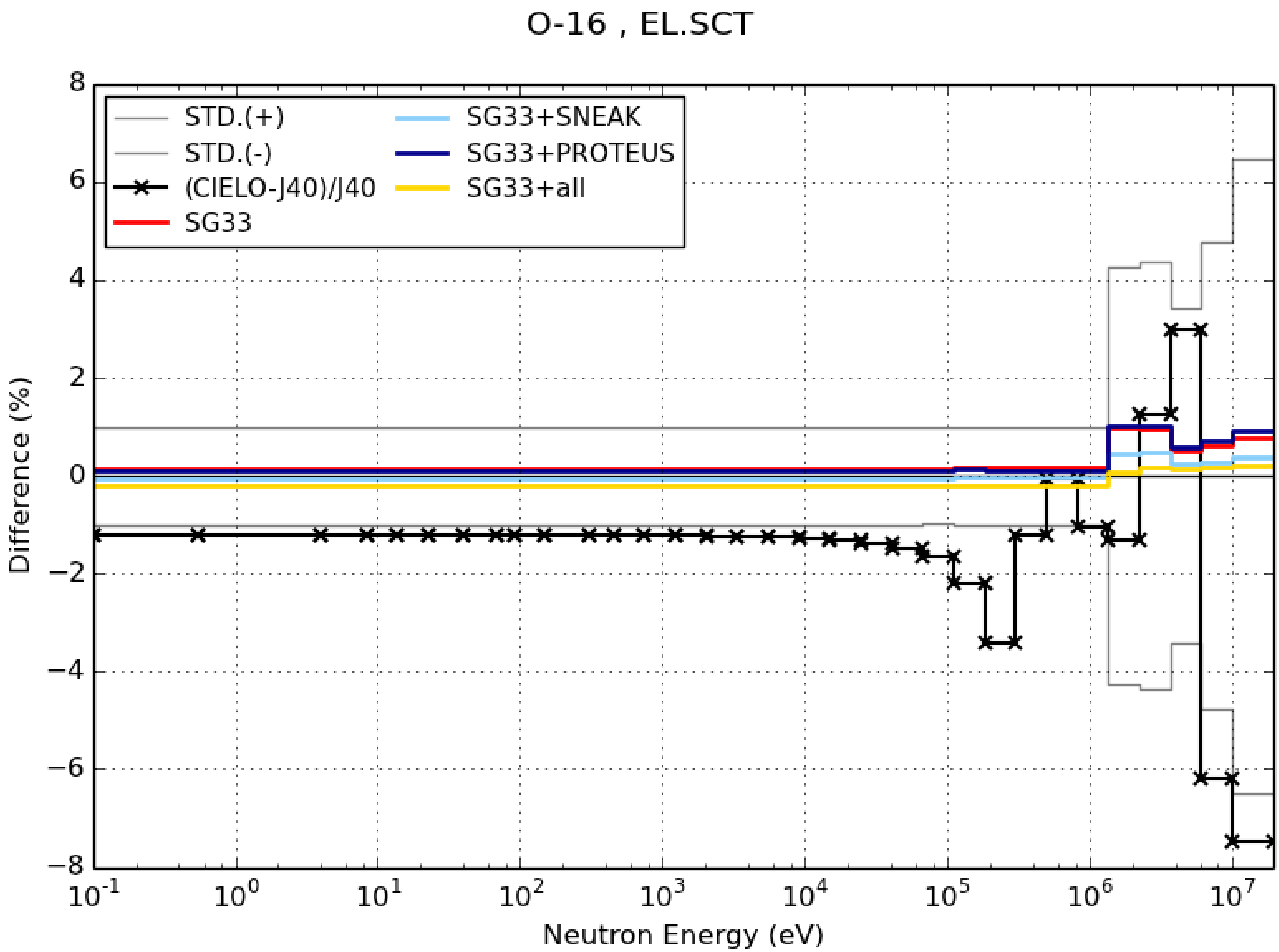
- All integral experiments increase Pu-239 capture cross section → There is no contradiction.

Pu-239 fission cross sections



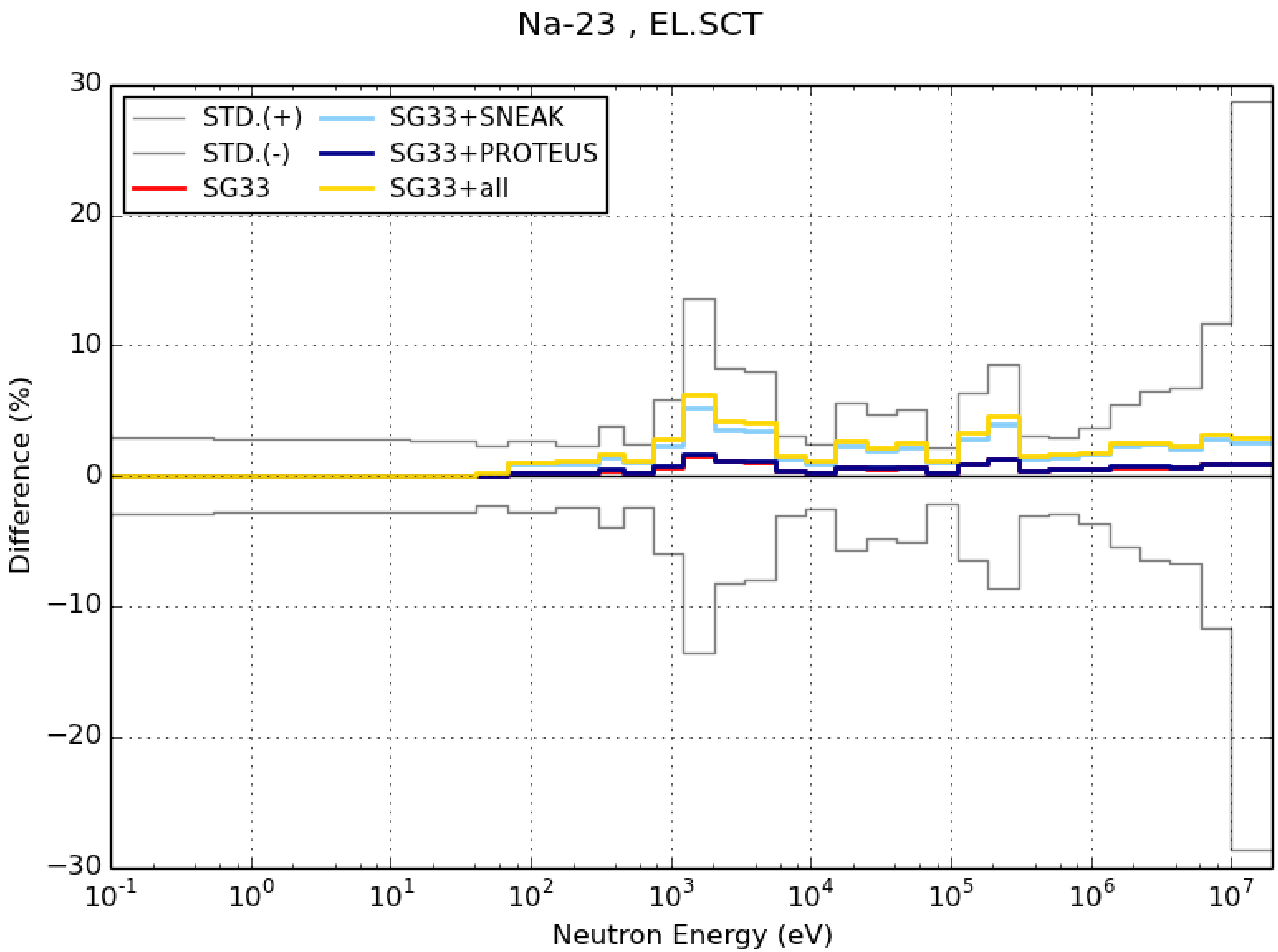
- The adjustment results of SG33, SG33+PROTEUS, and SG33+SNEAK seem to be consistent.

O-16 elastic scattering cross sections



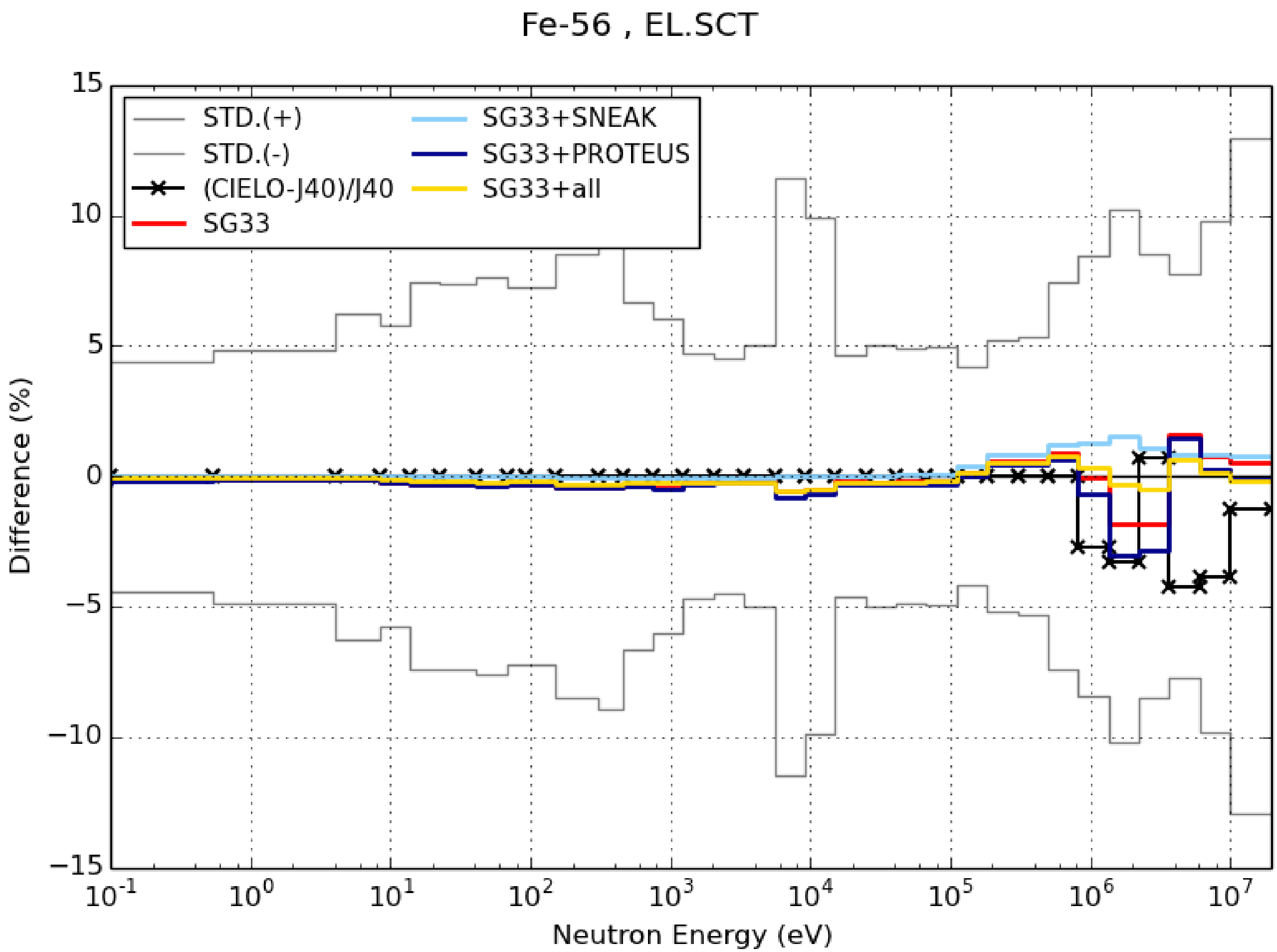
- The adjustment results have the similar trend with the evaluation of CIELO but the adjustments are quantitatively small.

Na-23 elastic scattering cross sections



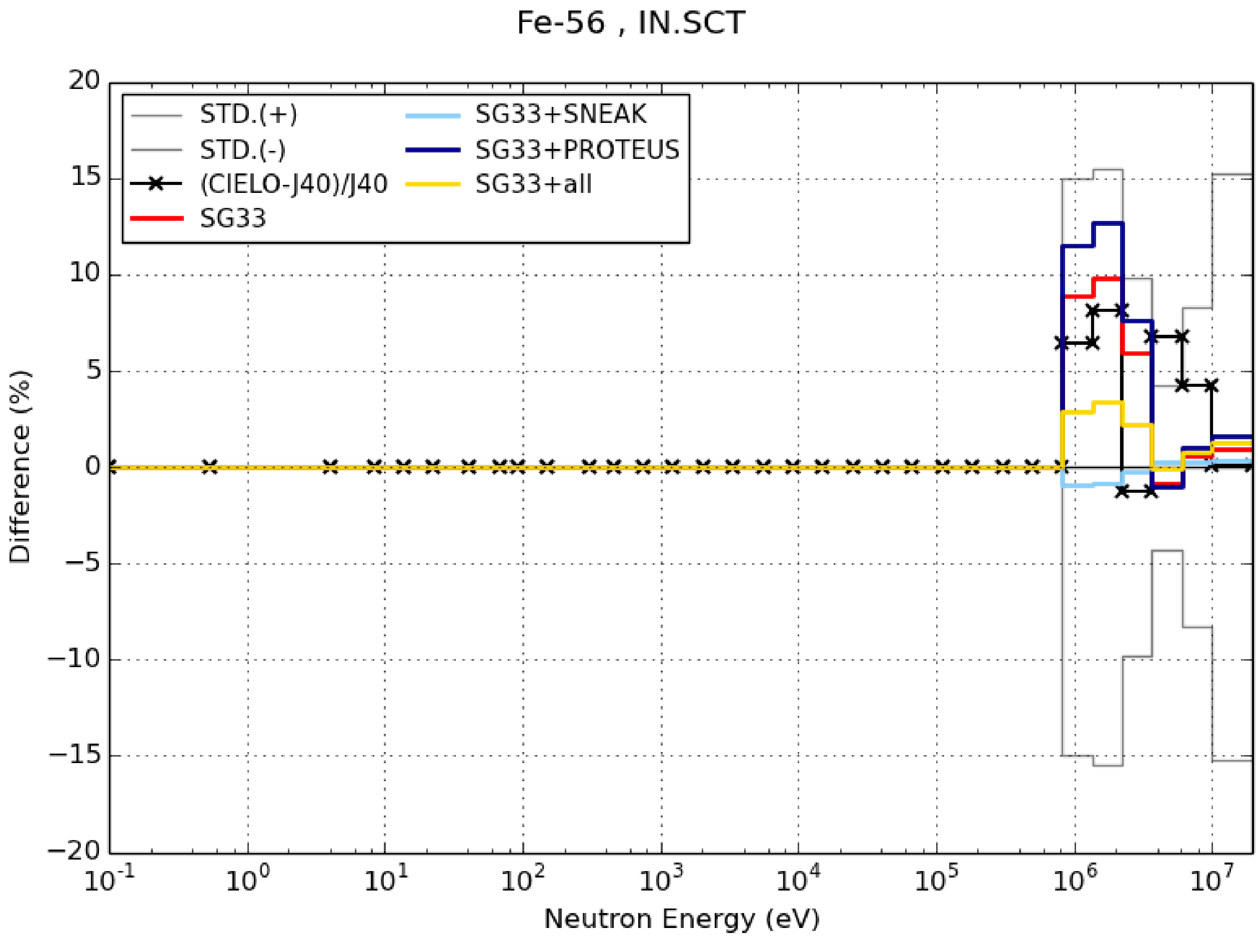
- All integral experiments increase Na-23 elastic scattering cross section → There is no contradiction.

Fe-56 elastic scattering cross sections



- Overcoming the problem of compensation effects, could we say that these adjustment results in MeV range support Fe-56 elastic scattering cross sections of CIELO?

Fe-56 inelastic scattering cross sections



- Again, could we say that these adjustment results in MeV range support Fe-56 inelastic scattering cross section of CIELO?
- We should carefully use these results when giving feedbacks to the evaluation of CIELO.

Concluding Remarks

- The result presented here is a model case of the methodology of CIELO verification by using cross-section adjustment technique, and the methodology itself seems to be very promising.

- However, we should be cautious about reflecting this cross-section adjustment results directly on the CIELO evaluation, since the integral experimental data applied here are quite limited.

- If we apply this methodology to much more comprehensive integral experimental data set and carefully determine the compensation effect, we would be able to provide useful information to CIELO in the future.

Appendix

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

HCLWR-PROTEUS

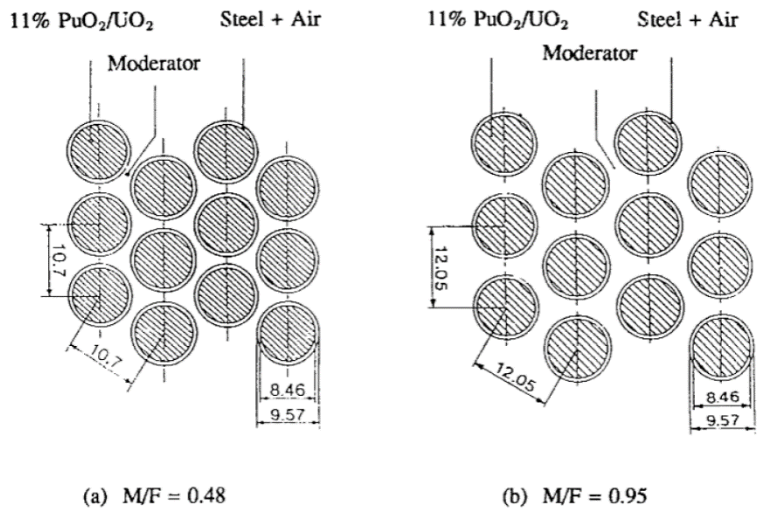
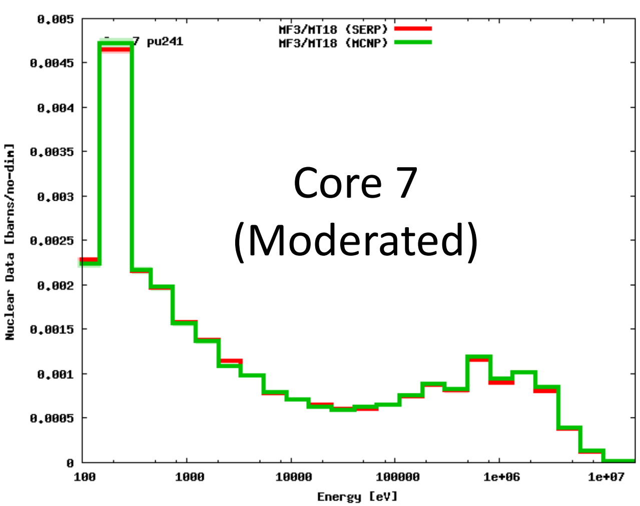
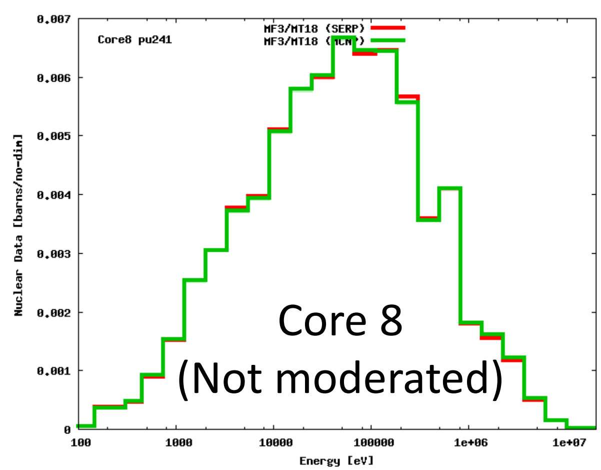


Fig.: Lattice description of the a) tight- and b) wide-pitch configuration*

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%





*: 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)

Fig.: Differential sensitivity of Pu-241 fission*

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

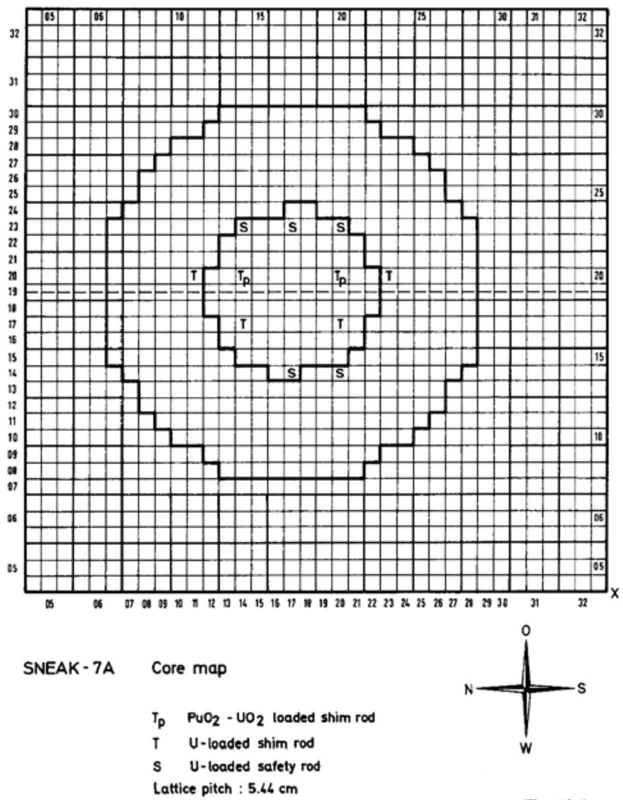


Fig.: SNEAK-7A Core Map*

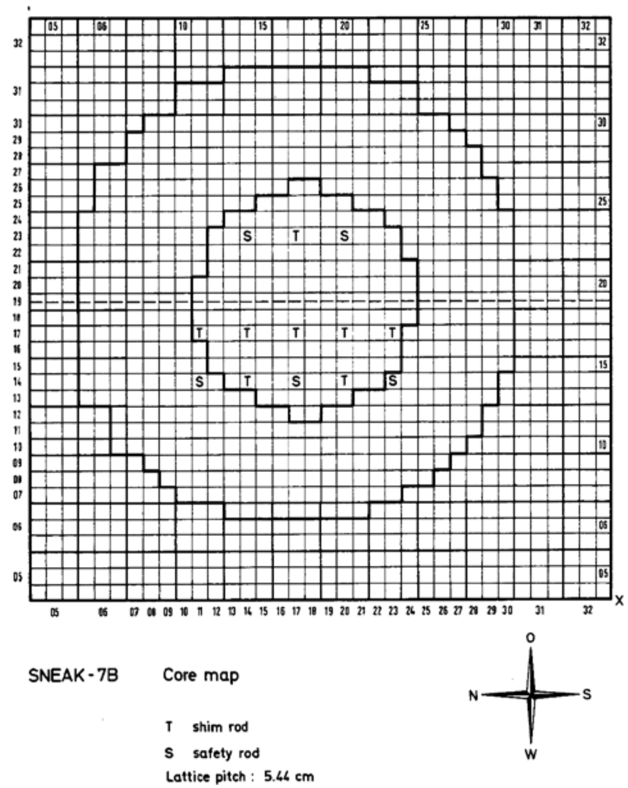


Fig.: SNEAK-7B Core Map*

*: 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	1.006497	1.0010 +- 0.0029	1.00549 +- 0.0029
SNEAK-7B KEFF	1.005863	1.0016 +- 0.0035	1.00426 +- 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 = 1.00549 → 1.01001)
  - Core 8: +0.503% (C/E = 1.00426 → 1.00929)