3rd Meeting of WPEC Subgroup 33 on
Methods and issues for the combined use of integral experiments and covariance data

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Proposal for How to Determine Error Matrix of Integral Data

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Discussion Points

- **What kind of errors needed in the adjustment?**
- **Error matrix of integral experiments?**
- **Error matrix of analytical modeling ?**

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'***

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

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

- Prediction error induced by the cross-section errors

  Before adjustment: GMG^t After adjustment: $GM'G^t$

✓**We need *Ve* as matrix form,**

✓**and, *Vm* as matrix form.**

Where, T_0 : Cross-section set before adjustment
M : Covariance before adjustment
Re : Measured values of integral experiments
Rc : Analytical values of integral experiments
Ve : Experimental errors of integral experiments
Vm : Analytical modeling errors of integral experiments
G : Sensitivity coefficients, $(dR/R)/(d\sigma/\sigma)$

Proposal for How to Determine Error Matrix of Integral Experimental Data

- **(Step 1)** Evaluate the components of the experimental errors for "Data A" and "Data B" quantitatively, and distinguish them into **Random errors (i.e., *independent errors* ($|\rho| = 0$)*between Data A and B*)**, or **Systematic errors (i.e., *common errors* ($|\rho| = 1$) *between Data A and B*)**. If an error component cannot be systematic or random either, divide the error to more detailed subcomponent until the component becomes either.
- **(Step 2)** Sum up of the experimental errors of Data A and B with **Random (σ_{Random})** and **Systematic ($\sigma_{Systematic}$)** components.
- **(Step 3)** Calculate the total error value and correlation factor:

$$Total\ error\ of\ Data\ A\ :\ \sigma_{Total,A} = \pm\sqrt{\sigma^2_{Random,A} + \sigma^2_{Systematic,A}}\ ,\quad \sigma_{Total,B} = \pm\sqrt{\sigma^2_{Random,B} + \sigma^2_{Systematic,B}}$$

$$Correlation\ \ factor\ between\ Data\ \ A\ and\ \ B\ :\ \rho_{A,B} = \frac{\sigma_{Systematic,A} \times \sigma_{Systematic,B}}{\sigma_{Total,A} \times \sigma_{Total,B}}$$

Example to Prepare Error Matrix of integral Experiment Data (Case 1: ZPPR-9 Na Void Reactivity)

Table 2.12. Summary of Uncertainties in the Zone Sodium Void Measurement in ZPPR-9.

Source of Uncertainty				Uncertainty		Random error	Systematic error
				cents	% of measured reactivity [a]		
Measurement technique	MSM method	Rod drop method	Counting statistics		+/-(0.2) [b]	0.2 % for Step3 and Step5	
			λi and $\beta i/\beta$		+/-1.0		1.0 % for Step3 and Step5
		$\frac{R_1 \cdot \varepsilon_2}{R_2 \cdot \varepsilon_1}$			+/-0.2	0.2 % for both step	
		$\frac{\beta_{eff,1}}{\beta_{eff,2}}$		negligible		0.0 % for both step	
		$\frac{S_{eff,2}}{S_{eff,1}}$			+/-0.5	0.5 % for both step	
	Adjustment	Interface gap		+/-0.03		Step3: 0.10 %, Step5: 0.09 %	
		Temperature		+/-0.27		0.09 % for both step	
		Pu decay		+/-0.0015		0.00 % for both step	
Geometry		Interface gap (included in adjustment of measurement technique)			--	0.0 % for both step	
Composition	Assumed deviation of material mass	Pu mass			Depend on measured void zones (see Table 2.10(1))		Step3: 0.72 %, Step5: 0.67 %
		U mass				1.0 % for both step	
		Stainless steel weight					
		Sodium mass					0.16 % for both step
		O mass				(Sub total) Step3: 1.16 %, Step5: 1.16 %	(Sub total) Step3: 1.24 %, Step5: 1.21 %
		C mass					
		^{239}Pu isotope ratio					
		^{235}U isotope ratio					
	Removed sodium mass				+/-1.0		
	Difference of stainless steel weight between the sodium-filled plates and the empty plates				+/-0.16		

(a) Every value in this column depends on the individual measurement case and is a relative uncertainty.

(b) Generalized uncertainty, refer the actual uncertainties presented in Table 1.13 and Table 1.14).

Table 1.13. Results of Zone Sodium-voiding Measurements in ZPPR-9.
(Ref. "ZPPR-11 Monthly Report for February 1980", ZPR-TM-361, Argonne National Laboratory (Feb. 1980).)

Step No.	Total Zone Size, Drawers	Zone Depth, mm	Total Na Mass,[a] kg	Reactivity Change,[b] cent		Reactivity Adjustment,[c] cent
				Cumulative +/- σ_m (σ_t)	Step +/-σ_m (σ_t)	
1	9	203.2	2.90	3.03+/-0.05 (0.10)	3.03+/-0.05 (0.10)	-0.04
2	37	203.2	11.94	11.56+/-0.04 (0.19)	8.53+/-0.06 (0.17)	-1.36
3	97	203.2	31.30	29.39+/-0.02 (0.36)	17.83+/-0.04 (0.32)	1.22
4	97	406.4	62.60	37.26+/-0.01 (0.43)	7.87+/-0.02 (0.10)	0.84
5	97	508.0	77.88	31.68+/-0.02 (0.36)	-5.58+/-0.04 (0.15)	0.13
6	97	685.8	105.11	24.44+/-0.03 (0.29)	-7.24+/-0.04 (0.15)	-0.82
Off-center Zones[d]						
1	25 (x axis)	203.2	8.07	0.93+/-0.06 (0.12)		
2	25 (y axis)	203.2	8.07	0.20+/-0.06 (0.12)		

(a) A random uncertainty of 1% is assigned to any mass or mass difference.
(b) Counting statistics only are included in σ_m. The value of σ_t includes uncertainties in the reactivity adjustment and a 1.1% uncertainty in the detector calibration as well as the counting statistics uncertainty.
(c) Prior to the measurement of the sodium-voided state, replacement of specified fuel drawers with sodium–voided is necessary. This adjustment accounts for differences in experimental conditions between the reference and the particular step. Namely, the reactivity change caused by interface gap, core temperature, Pu decay, and operational control rods are adjusted to the measured sodium-void reactivity. An uncertainty is assigned based on the magnitude of the adjustment.
(d) Outer core zones in Table 1.25.

(Total error) Step3: 1.70 %, Step5: 1.68 %

$$\rho(between\ Step3\ and\ Step5) = \frac{\sigma_{Systematic}(Step3) \times \sigma_{Systematic}(Step5)}{\sigma_{Total}(Step3) \times \sigma_{Total}(Step5)} = 0.53$$

Example to Prepare Error Matrix of integral Experiment Data (Case 2: ZPPR-9 Reaction Rate Ratio)

Table 2.22. Uncertainties Assigned to the Detector Calibration (Reference 6).

Typical Uncertainty (% of measured reaction rate)						
Reaction Rate				Reaction Rate Ratio		
^{239}Pu(n, f)	^{235}U(n, f)	^{238}U (n, f)	^{238}U(n, γ)	^{235}U(n, f)/ ^{239}Pu(n, f)	^{238}U (n, f)/ ^{239}Pu(n, f)	^{238}U(n, γ) / ^{239}Pu(n, f)
1.5	1.3	1.9	1.0	1.0	1.8	1.2

Table 2.26. Combined Uncertainties of Mapping Foil Data.

	Typical Uncertainty (% of measured reaction rate)							
	^{239}Pu fission		^{235}U fission		^{238}U fission		^{238}U capture	
	Core	Radial Blanket	Core	Radial Blanket	Core	Radial Blanket	Core	Radial Blanket
Measurement technique	1.3 [a]		1.1 [a]		1.7 [a]		1.0 [a]	
Geometry	negligible	--	negligible	1.0	negligible	0.1	negligible	0.9
Composition	0.18	---	0.17	0.08	0.22	0.27	0.18	0.06
Total	1.3	1.3	1.1	1.5	1.7	1.7	1.0	1.3

(a) see Table 2.19.

Table 2.27. Combined Uncertainties of Reaction Rate Ratio. (in core region)

			Typical Uncertainty (% of measured reaction rate ratio)					
			F25/F49		F28/F49		C28/F49	
			F25	F49	F28	F49	C28	F49
Measurement technique	Mapping foil		1.1	1.3	1.7	1.3	1.0	1.3
		Sub-total	1.7		2.1		1.6	
	Detector calibration		1.0 [a]		1.8 [a]		1.2 [a]	
Geometry			negligible		negligible		negligible	
Composition			0.06		0.22		0.05	
Total			2.0		2.8		2.0	

(a) see Table 2.22.

In ZPPR-9, the reaction rates were measured in the same run and at the same foil place.

Assume the systematic error of two reaction rate ratios (e.g. F49/F25 & F28/F25) come from the error of the common reaction rate (F25).

Reaction Ratio		F28/F25	F49/F25	C28/F25
Total Error		2.7%	2.0%	1.9%
Correlation factor	F28/F25	1.0	Symmetric.	
	F49/F25	0.23	1.0	
	C28/F25	0.23	0.32	1.0

Additional Experimental Information 1

(Ref: ICSBEP2009 DVD)

The issue is the uncertainty in the translation from the heterogeneous assembly model to the homogeneous benchmark model. Because there is a strong correlation between the two calculations, the difference in the two calculations can have a much smaller uncertainty than either individual calculation. That is, the calculations for the transformation Δk value are based on the same code and on the same cross sections, with similar sensitivities of k_{eff} to the cross sections, and are thus highly correlated. The ensuing uncertainty in the transformation Δk is therefore assumed smaller by an order of magnitude, or $\pm 0.2\%\ \Delta k$. Adding in quadrature the uncertainties due to use of ENDF/B-V cross sections and the uncertainty of 0.06% from statistics in the two VIM calculations yields a total uncertainty in the transformation Δk of 0.21% Δk.

Table 33. Experimental and Benchmark-Model Eigenvalues.[a]

Measured k_{eff}	1.00093 ± 0.00003
Experiment k_{eff}	1.00051 ± 0.00087
Monte Carlo transformation of model	-0.0139 ± 0.0021
Benchmark-Model k_{eff}	0.9866 ± 0.0023

(a) Each uncertainty estimate is one standard deviation.

The keff error of ZPR6/Assembly7 should be:

$$\pm 0.23\ \%\Delta k$$

, including the extrapolation uncertainty estimation for the large transformation (-1.39 %dk) between detailed Monte Carlo model and simple 2D RZ homogeneous model.

Additional Experimental Information 2

(Ref: IRPhEP2009 DVD)

Composition of Fuel Plates in ZPR6/7

NEA/NSC/DOC(2006)1

Liquid Metal Fast Reactor - LMFR

ZPR-LMFR-EXP-001
CRIT-SPEC-REAC-RRATE

Table 1.4.24. Pu-U-Mo Dow Fuel Compositions.

Plate ID	Nominal Size (inches)[a]	^{Pu}[b] Mass(g)	Mo Mass(g)	^{241}Am[b] Mass(g)	U Mass(g)
Pu-U-Mo DOW (1/4x2x4)	0.25x2x4	123.8230	11.0777	0.8172	301.9836
Pu-U-Mo DOW (1/4x2x5)	0.25x2x5	156.5097	13.9032	0.9959	381.4410
Pu-U-Mo DOW (1/4x2x6)	0.25x2x6	188.8543	16.9709	1.2855	461.9838
Pu-U-Mo DOW (1/4x2x7)	0.25x2x7	221.2774	19.6754	1.4110	540.1691
Pu-U-Mo DOW (1/4x2x8)	0.25x2x8	254.6300	22.9605	1.6064	621.3367

(a) Outer clad dimensions.
(b) Masses of ^{241}Pu and ^{241}Am in the table correspond to January 1, 1977. ^{241}Pu and ^{241}Am masses are decay-corrected to the date of the measurement in all calculational models.

Table 1.4.25. Pu-U-Mo Dow Fuel Pu and U Isotopic Weight Percents.[a]

Isotope	Pu-U-Mo DOW (1/4x2x4)	Pu-U-Mo DOW (1/4x2x5)	Pu-U-Mo DOW (1/4x2x6)	Pu-U-Mo DOW (1/4x2x7)	Pu-U-Mo DOW (1/4x2x8)
^{238}Pu	0.0372	0.0311	0.0402	0.0326	0.0340
^{239}Pu	87.1050	87.2316	87.0382	87.2034	87.1611
^{240}Pu	11.6131	11.6167	11.6133	11.6123	11.6229
^{241}Pu	1.0733	0.9808	1.1261	1.0029	1.0232
^{242}Pu	0.1714	0.1398	0.1822	0.1489	0.1588
^{235}U	0.2199	0.2200	0.2201	0.2200	0.2200
^{238}U	99.7801	99.7800	99.7799	99.7800	99.7800

(a) Plutonium weight percents in the table correspond to January 1, 1977. ^{241}Pu and ^{241}Am masses are decay-corrected to the date of the measurement in all calculational models.

Same !

Composition of Fuel Plates in ZPPR-9, 10A

NEA/NSC/DOE(2006)1

Liquid Metal Fast Reactor - LMFR

ZPPR-LMFR-EXP-001
CRIT-SPEC-REAC-RRATE

Table 1.1.4. Pu-U-Mo Dow Fuel Compositions.

ID Number	Plate ID	Nominal Size (inches)[a]	^{Pu}[b] Mass(g)	Mo Mass(g)	^{241}Am[b] Mass(g)	U Mass(g)
1	Pu-U-Mo DOW (1/4x2x4)	0.25x2x4	123.8230	11.0777	0.8172	301.9836
2	Pu-U-Mo DOW (1/4x2x5)	0.25x2x5	156.5097	13.9032	0.9959	381.4410
3	Pu-U-Mo DOW (1/4x2x6)	0.25x2x6	188.8543	16.9709	1.2855	461.9838
4	Pu-U-Mo DOW (1/4x2x7)	0.25x2x7	221.2774	19.6754	1.4110	540.1691
5	Pu-U-Mo DOW (1/4x2x8)	0.25x2x8	254.6300	22.9605	1.6064	621.3367

(a) Outer clad dimensions.
(b) Masses of ^{241}Pu and ^{241}Am in the table correspond to January 1, 1977

Table 1.1.5. Pu-U-Mo Dow Fuel Pu and U Isotopic Weight Percents.[a]

ID Number	1	2	3	4	5
Isotope	Pu-U-Mo DOW (1/4x2x4)	Pu-U-Mo DOW (1/4x2x5)	Pu-U-Mo DOW (1/4x2x6)	Pu-U-Mo DOW (1/4x2x7)	Pu-U-Mo DOW (1/4x2x8)
^{238}Pu	0.0372	0.0311	0.0402	0.0326	0.0340
^{239}Pu	87.1050	87.2316	87.0382	87.2034	87.1611
^{240}Pu	11.6131	11.6167	11.6133	11.6123	11.6229
^{241}Pu	1.0733	0.9808	1.1261	1.0029	1.0232
^{242}Pu	0.1714	0.1398	0.1822	0.1489	0.1588
^{235}U	0.2199	0.2200	0.2201	0.2200	0.2200
^{238}U	99.7801	99.7800	99.7799	99.7800	99.7800

(a) Plutonium weight percents in the table correspond to January 1, 1977.

Additional Experimental Information 3

(Ref: P. J. Collins, "Integral Experiment Information for Fast Reactors," Advances in Nuclear Science and Technology, Chap.4, Plenum Press, 1982)

TABLE VI

Covariance Matrices for CSEWG Benchmarks

	Experiment	Std Dev.,%	1	2	3	4	5	6	7	8	9	10	11	12	13	14
	ZPR-3/48		1	2	3	4										
1	k	0.10	1	0	0	0										
2	$^{28}c/^{25}f$	4.4			0.53	0										
3	$^{28}f/^{25}f$	4.6			1	0										
	ZPR-6/6A															
4	k	0.10				1										
5	$^{28}c/^{25}f$	2.7														
6	$^{28}f/^{25}f$	2.8					1	0	0	0.48	-0.23		0	0	0.37	-0.26
	ZPR-6/7															
7	k	0.10					1	0	0	0			0	0	0	0
8	$^{28}c/^{49}f$	2.3						1	0.24	0.40			0	0.21	0.12	0.13
9	$^{28}f/^{49}f$	2.9							1	0.34			0	0.04	0.57	0.24
10	$^{25}f/^{49}f$	2.1								1			0	0.05	0.24	0.53
	ZPR-9/31															
11	k	0.10											1	0	0	0
12	$^{28}c/^{49}f$	2.3												1	0.17	0.19
13	$^{28}f/^{49}f$	2.6													1	0.46
14	$^{25}f/^{49}f$	2.4														1

Note that measurements of criticality in the various configurations are assumed to be uncorrelated with each other and with reaction rates measured in the same or different assemblies.

In the benchmark data, reaction rate ratios usually are derived for a common denominator reaction rate. This leads to a strong correlation for reaction rates in the same assembly. For example, consider $^{25}f/^{49}f$ and $^{28}f/^{49}f$. Assuming for the moment that the measurements have no common uncertainty components, and let σ_9 be the standard deviation of ^{49}f, etc., we have

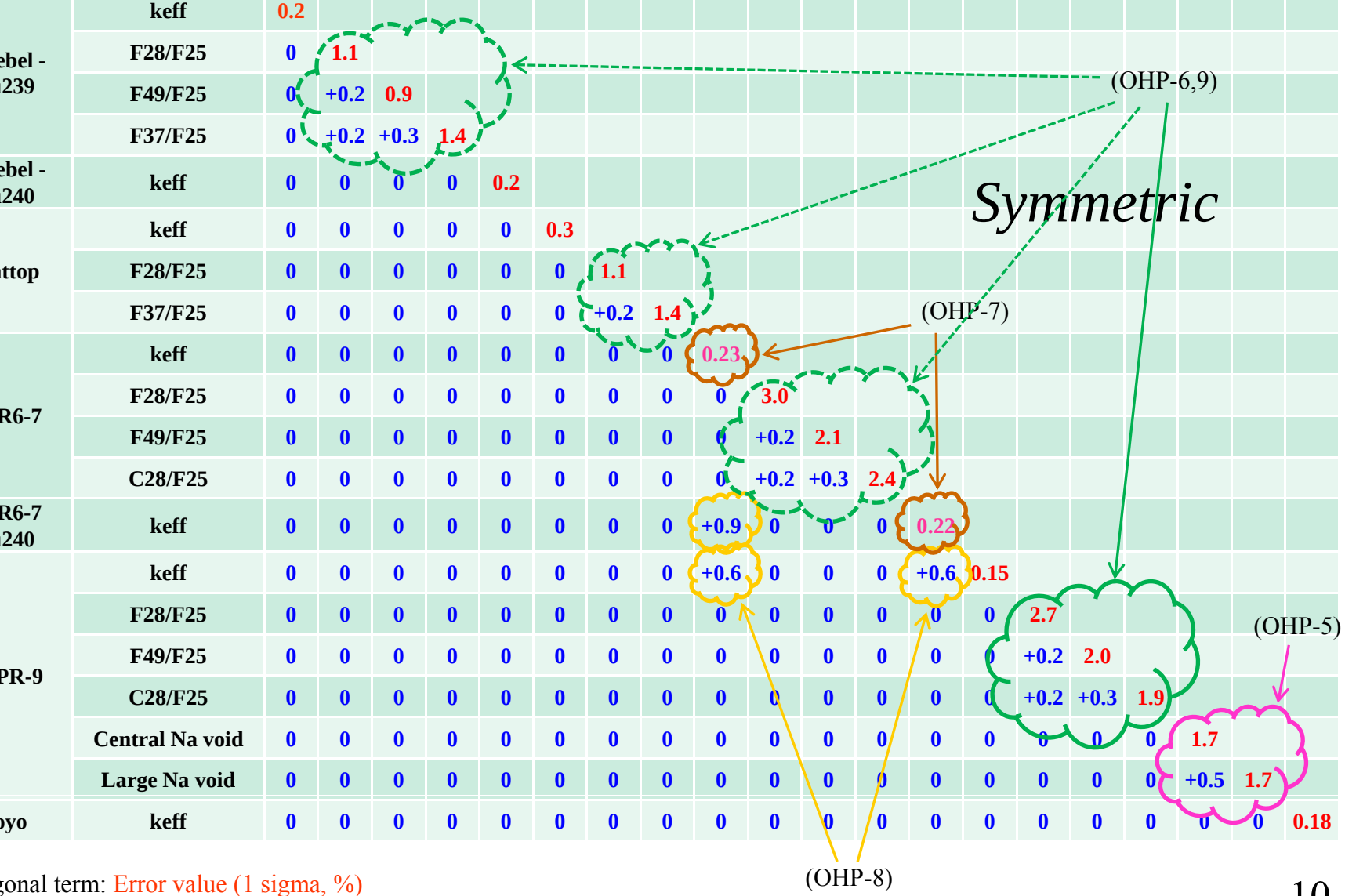
$$\rho(^{25}f/^{49}f,\ ^{28}f/^{49}f) = \sigma_9^2\,(\sigma_8^2 + \sigma_9^2)^{-\frac{1}{2}}(\sigma_5^2 + \sigma_9^2)^{-\frac{1}{2}} \qquad (16)$$

Then, for example, if the standard deviations are all equal,

$$\rho = 0.5 \qquad (17)$$

Proposal for Matrix *Ve* (Experimental Error)

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	+0.2	0.9																	
4		F37/F25	0	+0.2	+0.3	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	+0.2	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	+0.2	2.1									
12		C28/F25	0	0	0	0	0	0	0	0	0	+0.2	+0.3	2.4								
13	ZPR6-7 Pu240	keff	0	0	0	0	0	0	0	0	+0.9	0	0	0	0.22							
14	ZPPR-9	keff	0	0	0	0	0	0	0	0	+0.6	0	0	0	+0.6	0.15						
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	+0.2	2.0				
17		C28/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+0.2	+0.3	1.9			
18		Central Na void	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.7		
19		Large Na void	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+0.5	1.7	
20	Joyo	keff	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.18



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

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

Proposal for How to Determine Error Matrix of Analytical Modeling Method

➢**(Definition)** Analytical modeling errors which are **included in the calculation values**, besides contribution from nuclear data covariance.

➢**(For Continuous Energy Monte Carlo method with as-built model)** **Only statistical errors with no correlations.** However the most of MC codes estimate errors with considering no correlations.

* Correlation between integral parameters estimated in the same MC run. (ex. reaction rate ratio)
* Correlation between generations (cycles) for eigenvalue calculations.

For the latter case, the apparent (classical) variances are **always smaller** than the real ones, though the degree of underestimation depends on problems.

➢**(For Deterministic method with as-built model)** **Estimation from the sensitivity to approximation details of the models** such as transport effect, mesh-size effect, ultra-fine energy group effect, Sn-Pn order effect, etc. Note that these analytical modeling errors must be considered, even if the correction factors by the detailed modeling were applied to the final calculation result. See **Sugino's example**.

Concluding Remarks

- **JAEA would like to establish the standard of methodology for error matrix evaluation needed in this SG33 activity.**
  - **Covariance of nuclear data (or group constants), <- out of scope (later),**
  - **Standard deviations and their correlations of integral experiments,**
  - **Standard deviations and their correlations of analytical modeling.**

- **Error matrix of integral experiments.**
  - **Components of errors (measurement, geometry, and composition),**
  - **Characteristics of each error component (statistical, or systematic),**
  - **Determination of absolute error values,**
  - **Determination of correlation factors in error matrix.**

- **Error matrix of analytical modeling.**
  - ✓ **Definition of analytical modeling errors (included in Calculation values besides contribution from nuclear data covariance),**
  - ✓ **Monte Carlo calculation (including only statistical error),**
  - ✓ **Deterministic calculation (affected by various approximations of neutron transport equation).**