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Detailed comparison of Progressive Incremental Adjustment (PIA) sequence results involving adjustments of spectral indices and coolant density effects on the basis of the SG33 benchmark NEA Nuclear Data Week, WPEC/SG-39



Experimental configurations with integral parameters part of the data assimilation

Configuration	Integral parameters
GODIVA	F28/F25, F49/F25, F37/F25
JEZEBEL-Pu239	F28/F25, F49/F25, F37/F25
ZPR6-7	F28/F25, F49/F25, C28/F25
ZPPR9	F28/F25, F49/F25, C28/F25, Na Void Step 3, Na Void Step 5

- F28, F25, F49, and F37: respectively used for ²³⁸U, ²³⁵U, ²³⁹Pu, and ²³⁷Np microscopic fission reaction rates per atom.
 C28: ²³⁸U capture reaction rate per ²³⁸U atom.
 All spectral indices, Table, at core center.
- Na Void Step 3 and Na Void Step 5: reactivity effects (ZPPR9) due to Na removal from small zone near core center and from leakage dominated larger configuration.
- 10 nuclides adjusted: ¹⁶O, ²³Na, ⁵²Cr, ⁵⁶Fe, ⁵⁸Ni, ²³⁵U, ²³⁸U, ²³⁹Pu, ²⁴⁰Pu, ²⁴¹Pu.



12 target configurations

Target experimental configurations with integral parameters

Integral parameters
F28/F25, F49/F25, F37/F25, k _{eff} ^(a)
F28/F25, F49/F25, F37/F25, k _{eff} ^(a)
F28/F25, F49/F25, C28/F25, k _{eff} ^(a)
F28/F25, F49/F25, C28/F25, Na Void Step 3, Na Void Step 5, k_{eff} ^(a)
k _{eff}
k _{eff}
k _{eff}
F28/F25, F37/F25, k _{eff}
F28/F25, F49/F25, F37/F25, k _{eff}
k _{eff}
k _{eff}
k _{eff}

^(a)Also part of the adjustment in one of the simulations.



- JEZEBEL-Pu240, ZPR6-7 Pu240, JOYO.
- FLATTOP-Pu: Pu sphere reflected by natural U.
- FLATTOP-25: ²³⁵U sphere reflected by natural U.
- MIX-MET-FAST-001: Pu sphere surrounded by highly enriched U.
- PU-MET-FAST-010: Pu sphere surrounded by Al.
- PU-MET-FAST-009: δ -phase Pu sphere reflected by natural U.



Sensitivity coefficients

• ERANOS (2.2-N), explicit, 33 group

by means of flux, adjoint flux, generalized importance.

• Generalized Perturbation Theory

(GPT) : spectral indices.

• Equivalent Generalized Perturbation Theory (EGPT): reactivity effects.

• [Standard Perturbation Theory (SPT) : k_{eff} , limited use.]



Iterative procedure used in individual incremental steps within PIA:

For i = 0, 1, 2, ... i = 0: a priori, starting point:

$$\Delta T_{i} = M_{i}G_{i}^{T}\left(G_{i}M_{i}G_{i}^{T} + V_{E} + V_{M}\right)^{-1}CE_{i} , CE_{i} = \left(CE_{i,k}\right) = \left(\frac{R_{E,k} - (R_{c}(T_{i}))_{,k}}{(R_{c}(T_{i}))_{,k}}\right)$$
(1)

with

 $M_i = (M_{i,j,j'}) = cov(T_{i,j}, T_{i,j'})/(T_{i,j}T_{i,j'})$: nuclear data variance/covariance matrix in relative terms.

i = 0: M_0 : derived from COMMARA-2.0, this study.

$$M_{i+1} = (M_{i+1,j,j'}) = M_i - M_i G_i^T (G_i M_i G_i^T + V_E + V_M)^{-1} G_i M_i$$
⁽²⁾



Additionally, Eq. (1):

$$\Delta T_{i} = \left(\Delta T_{i,j}\right) = \left(\frac{T_{i+1,j} - T_{i,j}}{T_{i,j}}\right) = \left(\frac{T_{i+1,j}}{T_{i,j}} - 1\right) = \left(F_{i,j} - 1\right) \implies$$

$$T_{i+1} = \left(T_{i+1,j}\right) = \left(T_{i,j}F_{i,j}\right), \qquad F_{i} = \left(F_{i,j}\right) = \left(1 + \Delta T_{i,j}\right) \qquad (3)$$

 $T_i = (T_{i,j})$: data set vector. Starting from JEFF-3.1, this study.

 $R_C(T_i) = ((R_C(T_i))_{,k})$: analytical values vector. Through ERANOS (2.2-N), this study. PIA: for integral parameters k dealt with in specific step.

- $F_i = (F_{i,j})$: adjustment factor vector i.e. $T_{i+1,j} = (\prod_{m=0}^{i} F_{m,j})T_{0,j}$.
- $R_E = (R_{E,k})$: vector of the central values of the experimental integral parameters.



$$G_i = (G_{i,k,j}) = \left(\frac{d\left((R_c(T_i))_{,k}\right)}{(R_c(T_i))_{,k}} \middle/ \frac{dT_{i,j}}{T_{i,j}}\right)$$

: in the form of sensitivity coefficient vector by using appropriate indexing.

 $V_E = (V_{E,k,k'}) = cov(R_{E,k}, R_{E,k'}) / (R_{E,k}R_{E,k'}) : \text{experimental variance/covariance}$ matrix.

$$V_{M} = (V_{M,k,k'}) = cov \left((R_{c}(T))_{,k}, (R_{c}(T))_{,k'} \right) / \left((R_{c}(T))_{,k} (R_{c}(T))_{,k'} \right)$$

: analytical modeling matrix.



From iteration i to i + 1, two steps:

(1)
$$M_i, G_i, V_E, V_M, R_E, R_C(T_i) \xrightarrow{\text{Eq. 1}} \Delta T_i \xrightarrow{\text{Eq. 3}} F_i, T_{i+1}$$
 In house
 $M_i, G_i, V_E, V_M \xrightarrow{\text{Eq. 2}} M_{i+1}$ In house

(2) In house tool MICADJ ERANOS (2.2-N) $\Rightarrow R_C(T_{i+1}), G_{i+1};$ together with M_{i+1} : go to (1)

and replace i by i + 1.

(1), (2) until $F_n = 1 \rightarrow n$ iterations needed to converge. Practical reason: $0.99 < F_{n,j} < 1.01$, this study.



Adjustment: this study, 6 cases

• Simulation 1: integral parameters assimilated simultaneously.

PIA: Simulations 2, 2A, 2B, 3, 3A, 3B:

• 2:

GODIVA spectral indices \rightarrow ZPPR9 coolant density effects \rightarrow ZPPR9 spectral indices \rightarrow ZPR6-7 spectral indices \rightarrow JEZEBEL-Pu239 spectral indices.

- 2A: Simulation $2 \rightarrow k_{eff}$ of the 4 configurations just for $\bar{\nu}$.
- 2B: Similar to Simulation 2: no iterations.
- 3 : Reversed order as compared to Simulation 2: JEZEBEL-Pu239 first.
- 3B: Similar to Simulation 3: no iterations.



A posteriori *C/E*s for target experiments

Configuration	Integral	Experimental	Simulation			_
	parameter	uncertainty	1	2	2A	3
		(%)	C/E			
	F28/F25	1.1	1.000	0.998	0.998	1.000
GODIVA	F49/F25	1.0	1.001	1.001	1.001	1.001
	F37/F25	1.4	1.000	0.996	0.996	1.000
	k_{eff}	0.1	0.976	0.977	0.998	0.977
	F28/F25	1.1	0.990	0.997	0.997	0.990
JEZEBEL-Pu239	F49/F25	0.9	0.998	0.999	0.999	0.998
	F37/F25	1.4	1.006	1.005	1.005	1.006
	k_{eff}	0.2	0.995	0.995	0.999	0.995
	F28/F25	3.0	1.030	1.020	1.021	1.037
ZPR6-7	F49/F25	2.1	0.982	0.977	0.977	0.977
	C28/F25	2.4	1.004	1.001	1.001	1.003
	k_{eff}	0.2	1.015	1.007	1.002	1.008
	F28/F25	2.7	0.979	0.951	0.951	0.971
	F49/F25	2.0	1.004	0.997	0.997	0.996
ZPPR9	C28/F25	1.9	0.996	0.994	0.994	0.996
	Na Void Step 3	1.9	1.020	1.033	1.031	1.034
	Na Void Step 5	1.9	0.985	0.975	0.972	0.979
	k_{eff}	0.1	1.013	1.006	1.000	1.007
JEZEBEL-Pu240	k_{eff}	0.2	1.000	0.999	1.006	0.999
ZPR6-7 Pu240	k_{eff}	0.2	1.012	1.007	1.002	1.008
JOYO	k_{eff}	0.2	0.998	0.993	0.999	0.994
	F28/F25	1.1	0.954	0.981	0.983	0.978
FLATTOP-Pu	F37/F25	1.4	0.990	1.004	1.006	1.002
	k_{eff}	0.3	1.013	0.991	0.992	0.995
	F28/F25	1.1	0.983	0.996	0.998	0.994
FLATTOP-25	F49/F25	0.9	1.003	1.005	1.005	1.004
	F37/F25	1.3	1.000	1.005	1.006	1.003
	k_{eff}	0.1	0.990	0.972	0.988	0.976
MIX-MET-FAST-001	k_{eff}	0.2	0.994	0.993	1.000	0.993
PU-MET-FAST-010	k_{eff}	0.2	0.992	0.985	0.987	0.987
PU-MET-FAST-009	k_{eff}	0.3	0.990	0.988	0.991	0.988



A posteriori *C/Es* for target experiments

Configuration	Integral	Experimental	Simulation		
	parameter	uncertainty	2B 3B		•
		(%)	C/E		
	F28/F25	1.1	0.991	0.991	
GODIVA	F49/F25	1.0	0.994	0.994	
	F37/F25	1.4	0.995	0.995	
	k_{eff}	0.1	0.978	0.978	
	F28/F25	1.1	0.990	0.991	
JEZEBEL-Pu239	F49/F25	0.9	0.994	0.994	
	F37/F25	1.4	1.010	1.011	
	k_{eff}	0.2	0.991	0.991	
	F28/F25	3.0	1.033	1.036	
ZPR6-7	F49/F25	2.1	0.969	0.969	
	C28/F25	2.4	1.004	1.004	
	k _{eff}	0.2	1.012	1.012	
	F28/F25	2.7	0.976	0.979	
	F49/F25	2.0	0.989	0.990	
ZPPR9	C28/F25	1.9	0.996	0.995	•
	Na Void Step 3	1.9	1.042	1.041	
	Na Void Step 5	1.9	0.984	0.984	
	k_{eff}	0.1	1.005	1.005	
JEZEBEL-Pu240	k_{eff}	0.2	0.996	0.996	
ZPR6-7 Pu240	k_{eff}	0.2	1.006	1.006	•
JOYO	k_{eff}	0.2	0.993	0.993	
	F28/F25	1.1	0.957	0.956	
FLATTOP-Pu	F37/F25	1.4	0.996	0.995	
	k_{eff}	0.3	1.001	1.002	
	F28/F25	1.1	0.985	0.985	
FLATTOP-25	F49/F25	0.9	0.997	0.997	
	F37/F25	1.3	1.003	1.002	
	k _{eff}	0.1	0.977	0.978	
MIX-MET-FAST-001	k _{eff}	0.2	0.990	0.990	
PU-MET-FAST-010	k _{eff}	0.2	0.983	0.983	
PU-MET-FAST-009	k _{eff}	0.3	0.992	0.993	

Spectral indices: within experimental uncertainty or just slightly outside, most cases. Exception: some of the F28/F25s: maximum discrepancy 4σ . As expected: 2 and 2A similar results. 2B and 3B also similar.

Coolant density effects: discrepancy < 2σ .

k_{eff} :

improvement with 2A especially for configurations considered in assimilation.



A posteriori nuclear data uncertainties

Configuration	Integral	Experimental	Simulation				
	parameter	uncertainty	1	2	2A	3	
		(%)	Uncertainty (%)				
	F28/F25	1.1	0.2	0.6	0.6	0.5	
GODIVA	F49/F25	1.0	0.2	0.2	0.2	0.3	
	F37/F25	1.4	0.2	0.5	0.5	0.5	
	k_{eff}	0.1	0.6	0.7	0.7	0.7	
	F28/F25	1.1	0.5	0.3	0.3	0.4	•
JEZEBEL-Pu239	F49/F25	0.9	0.2	0.2	0.2	0.3	
	F37/F25	1.4	0.4	0.3	0.3	0.5	
	k_{eff}	0.2	0.3	0.3	0.2	0.3	
	F28/F25	3.0	0.5	0.9	0.9	0.7	
ZPR6-7	F49/F25	2.1	0.3	0.4	0.4	0.4	
	C28/F25	2.4	0.3	0.7	0.7	0.5	
	k_{eff}	0.2	0.5	0.6	0.5	0.5	
	F28/F25	2.7	0.4	1.2	1.2	0.7	
	F49/F25	2.0	0.3	0.4	0.4	0.4	
ZPPR9	C28/F25	1.9	0.3	0.7	0.7	0.5	
	Na Void Step 3	1.9	0.7	1.9	1.9	1.1	
	Na Void Step 5	1.9	0.8	2.2	2.2	1.3	
	k_{eff}	0.1	0.5	0.6	0.5	0.5	
JEZEBEL-Pu240	k_{eff}	0.2	0.5	0.5	0.4	0.5	
ZPR6-7 Pu240	k_{eff}	0.2	0.5	0.6	0.5	0.5	
JOYO	k_{eff}	0.2	0.8	0.9	0.8	0.9	
	F28/F25	1.1	0.5	0.4	0.3	0.4	
FLATTOP-Pu	F37/F25	1.4	0.5	0.4	0.4	0.5	
	k_{eff}	0.3	0.3	0.4	0.3	0.3	
	F28/F25	1.1	0.4	0.6	0.6	0.6	
FLATTOP-25	F49/F25	0.9	0.2	0.2	0.2	0.3	
	F37/F25	1.3	0.4	0.6	0.6	0.5	
	k _{eff}	0.1	0.8	0.9	0.9	0.9	
MIX-MET-FAST-001	k _{eff}	0.2	0.2	0.2	0.2	0.2	
PU-MET-FAST-010	k _{eff}	0.2	0.3	0.4	0.3	0.3	
PU-MET-FAST-009	k _{eff}	0.3	0.2	0.3	0.2	0.3	

- Spectral indices:
 - < experimental uncertainties.
- Coolant density effects:
 - \approx experimental uncertainties.

• k_{eff} :

- > experimental uncertainties
 (consistent with C/Es, several σs deviations).
- Simulation 1: smaller uncertainties.
- 2, 2A and 3 comparable.
 - $2B \approx 3B$, larger in most cases.



A posteriori nuclear data uncertainties

Configuration	Integral	Experimental uncertainty	Simulation	
	parameter	(%)	2B	3B
			Uncertainty (%)	
	F28/F25	1.1	0.9	0.9
GODIVA	F49/F25	1.0	0.5	0.5
	F37/F25	1.4	0.7	0.7
	k_{eff}	0.1	0.7	0.7
	F28/F25	1.1	0.8	0.8
JEZEBEL-Pu239	F49/F25	0.9	0.5	0.5
	F37/F25	1.4	0.6	0.6
	k_{eff}	0.2	0.4	0.4
	F28/F25	3.0	1.8	1.7
ZPR6-7	F49/F25	2.1	0.6	0.6
	C28/F25	2.4	1.1	1.1
	k_{eff}	0.2	0.6	0.6
	F28/F25	2.7	2.1	2.1
	F49/F25	2.0	0.6	0.6
ZPPR9	C28/F25	1.9	1.1	1.1
	Na Void Step 3	1.9	2.5	2.5
	Na Void Step 5	1.9	3.0	3.0
	k_{eff}	0.1	0.6	0.6
JEZEBEL-Pu240	k _{eff}	0.2	0.5	0.5
ZPR6-7 Pu240	k_{eff}	0.2	0.6	0.6
JOYO	k_{eff}	0.2	0.9	0.9
	F28/F25	1.1	0.7	0.7
FLATTOP-Pu	F37/F25	1.4	0.6	0.6
	k_{eff}	0.3	0.4	0.4
	F28/F25	1.1	0.9	0.9
FLATTOP-25	F49/F25	0.9	0.5	0.5
	F37/F25	1.3	0.8	0.8
	k_{eff}	0.1	0.9	0.9
MIX-MET-FAST-001	k_{eff}	0.2	0.3	0.3
PU-MET-FAST-010	k_{eff}	0.2	0.5	0.5
PU-MET-FAST-009	k_{eff}	0.3	0.4	0.4
		-		



Adjustment of the ²³⁹Pu inelastic scattering cross-section with respect to JEFF-3.1 a priori data in 33 groups



Adjustment: strong, max. 1σ COMMARA-2.0.

- $2 \equiv 3$; $2B \equiv 3B$: sequence independent.
- $2 \neq 2B$: important role of iterations.

 10^{6}

1 similar to 2,

smaller magnitude: compensations.

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Adjustment of the ²³⁹Pu elastic scattering cross-section



Adjustment, PIA:JEZEBEL-Pu239.



Adjustment of the ²³⁹Pu capture cross-section



- 2 ≡ 3. 2B ≡ 3B.
- 2 ≠ 2B ≠ 1.





- Fission source range: JEZEBEL-Pu239.
- Near main Na resonance 2.85keV: ZPR6-7.
- ZPPR9: seems unimportant or redundant.





Adjustment of the ²³⁹Pu fission cross-section



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Adjustment of the ²³⁵U inelastic scattering cross-section



GODIVA.



Adjustment of the ²³⁵U elastic scattering cross-section





Adjustment of the ²³⁵U capture cross-section





Adjustment of the ²³⁵U fission cross-section



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Adjustment of the ²³⁸U inelastic scattering cross-section





Adjustment of the ²³⁸U elastic scattering cross-section





Adjustment of the ²³⁸U capture cross-section



- $2 \neq 3 \neq 1$.
- $2B \equiv 3B$: almost no adjustment.

Adjustment, weak:

Conflicting between ZPPR9 and ZPR6-7, PIA: ۰ unreliable.

U238 (n,capture) adjustment

U238 (n,capture) adjustment



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Adjustment of the ²³⁸U fission cross-section





Adjustment of the ²³Na inelastic scattering cross-section



- 2 ≠ 3 ≠ 1.
- 2B ≡ 3B.



• Conflicting between ZPPR9 and ZPR6-7, PIA.





Adjustment of the ²³Na elastic scattering cross-section



- E > 1MeV: 2 ≠ 3.
- E < 1MeV: 2 ≡ 3.
- 2B ≡ 3B.

Adjustment without PIA stronger, different trend.

- E > 1MeV: conflicting between ZPPR9 and ZPR6-7.
- E < 1MeV: ZPPR9 coolant density effects + ZPR6-7, PIA.





Additional stronger adjustments











• Divergence, "Tsunami" effect reversing trends \rightarrow Adjusting k_{eff} should be avoided.



- I. PIA, integral parameters to assimilate: spectral indices and local reactivity effects.
- II. PIA, reject adjustment for cross-section of given isotope, data type and energy group or range when:

Adjustment depends on sequence, inconsistent \leftrightarrow

- Conflicting effects between different steps.
- A posteriori sensitivity coefficients of the integral parameters to this cross-section also sequence dependent.



III. Conversely, PIA reliable adjustment:

Largely independent of sequence, consistent.

- Clear separation of effects coming from individual steps without inconsistencies: though some integral parameters may be unneeded in cases where their assimilation does not have any impact on the adjustment, redundancy.
- The a posteriori sensitivity coefficients to the cross section under study independent of the sequence.



IV. Limited data base, this study: ²³⁸U and ²³Na crosssections not adjustable. Needs considering additional experiments.