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Consistent adjustment on the basis of TENDL data: Sandro Pelloni and Dimitri Rochman

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This study:

- Data assimilation: 4 configurations + 14 integral experiments.
- 10 nuclides considered in adjustment:
  ^{16}O, ^{23}Na, ^{52}Cr, ^{56}Fe, ^{58}Ni, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu.
- New: 33 group TENDL based a priori cross-sections.

+

- New: 33 group a priori TENDL based variance/covariance data.

❖Compared:

TENDL / TENDL (consistent)
TENDL / COMMARA-2.0
Same xs
Different covs

JEFF-3.1 / COMMARA-2.0
TENDL / COMMARA-2.0
Different xs
Same covs

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Asymptotic Progressive Incremental Adjustment (APIA)

(Asymptotic: maximum cross-section change between iterations < 1%)

Configuration	Integral parameters to assimilate	
GODIVA	*F28/F25, F49/F25, F37/F25*	
JEZEBEL-Pu239	*F28/F25, F49/F25, F37/F25*	At core
ZPR6-7	*F28/F25, F49/F25, C28/F25*	center
ZPPR9	*F28/F25, F49/F25, C28/F25,* Na Void -Step 3, -Step 5: coolant density effects	

- **APIA-1**: GODIVA spectral indices → ZPPR9 coolant density effects → ZPPR9 spectral indices → ZPR6-7 spectral indices → JEZEBEL-Pu239 spectral indices.
- **APIA-2**: JEZEBEL-Pu239 spectral indices → ZPR6-7 spectral indices → ZPPR9 spectral indices→ ZPPR9 coolant density effects → GODIVA spectral indices (reversed).

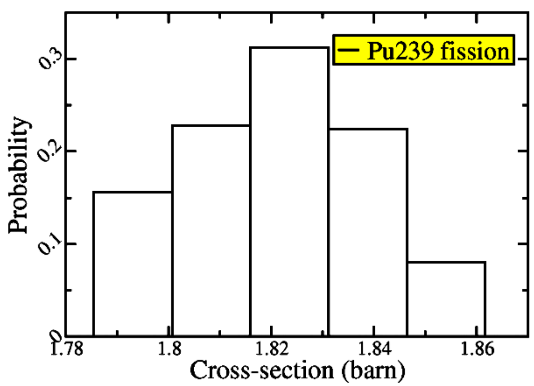
TENDL data source and target experiments

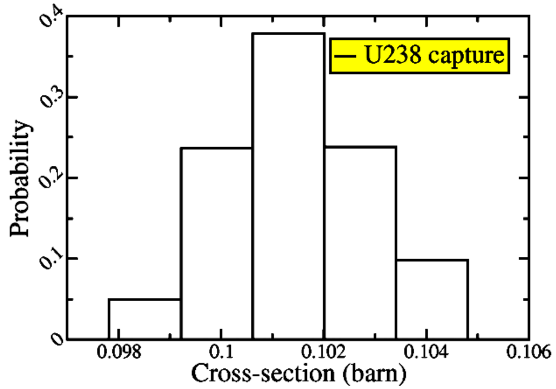
Nuclide	TENDL Edition
^{16}O	2016
^{23}Na	2017
^{52}Cr	2012
^{56}Fe	2012
^{58}Ni	2012
^{235}U	2014
^{238}U	2013
^{239}Pu	2013
^{240}Pu	2016
^{241}Pu	2012

Configuration	Integral parameter	Part of the data assimilation (Yes/No)
GODIVA	*F28/F25*, *F49/F25*, *F37/F25*	Yes
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	
FLATTOP-Pu	*F28/F25*, *F37/F25*	No
FLATTOP-25	*F28/F25*, *F49/F25*, *F37/F25*	

TENDL data

- Random ENDF-formatted Files ($N = 500$ per nuclide, sufficient): TALYS.
- Processed with NJOY (2012.21). IWT=8 in GROUPR.
- Probability distributions rather normal:





E.g. between 1.35 MeV and 0.83 MeV (Group 6)

- Expected values (mean)

Covariance data

ERANOS broad group libraries

$$d_m = \frac{1}{N}\sum_{i=1}^{N} d_{mi}$$

$m \in \{j, k\}$

$$cov(d_j, d_k) = \frac{1}{N-1}\sum_{i=1}^{N}(d_{ji} - d_j)(d_{ki} - d_k)$$

Results

Configuration	Integral parameter	Experimental uncertainty (%)	TENDL Data	APIA Simulation 1	APIA Simulation 2	APIA Simulation 1	APIA Simulation 2
				Covariance data: TENDL	TENDL	COMMARA-2.0	COMMARA-2.0
			A priori	A posteriori *C/E*			
GODIVA	*F28/F25*	1.1	0.929	1.001	0.999	0.999	0.996
	F49/F25	1.0	0.978	0.998	0.997	1.003	1.001
	F37/F25	1.4	0.961	0.986	0.984	1.000	0.996
JEZEBEL-Pu239	*F28/F25*	1.1	0.933	0.996	0.998	0.996	0.996
	F49/F25	0.9	0.981	1.002	1.002	0.999	0.999
	F37/F25	1.4	0.987	1.009	1.008	1.007	1.007
ZPR6-7	*F28/F25*	3.0	0.963	1.036	1.040	1.025	1.029
	F49/F25	2.1	0.960	0.984	0.981	0.978	0.979
	C28/F25	2.4	1.005	1.007	1.008	1.000	1.001
ZPPR9	*F28/F25*	2.7	0.909	0.978	0.982	0.968	0.972
	F49/F25	2.0	0.980	1.005	1.002	0.998	0.998
	C28/F25	1.9	0.997	1.000	1.001	0.993	0.995
	Na Void Step 3	1.9	1.140	1.034	1.038	1.045	1.035
	Na Void Step 5	1.9	1.113	0.994	0.999	1.011	1.001
FLATTOP-Pu	*F28/F25*	1.1	0.952	1.002	1.003	0.984	0.982
	F37/F25	1.4	1.005	1.023	1.022	1.017	1.016
FLATTOP-25	*F28/F25*	1.1	0.940	1.002	1.002	1.001	0.998
	F49/F25	0.9	0.984	1.003	1.001	1.008	1.006
	F37/F25	1.3	0.982	1.000	0.998	1.015	1.012

C/Es

- Mostly within experimental uncertainty.
  Na effect: < 2σ.
- Qualitatively consistent despite different covariances.
- Similar to JEFF-3.1/COMMARA-2.0 (previous study).
- Marked improvement as against a priori, especially *F28/F25*.

Uncertainties due to nuclear data uncertainties (TENDL based cross-sections)

Configuration	Integral parameter	Covariance data	
		TENDL	COMMARA-2.0
		A priori uncertainty (%)	
GODIVA	*F28/F25*	2.4	2.1
	F49/F25	1.8	0.7
	F37/F25	1.6	1.6
JEZEBEL-Pu239	*F28/F25*	2.4	2.4
	F49/F25	2.0	0.7
	F37/F25	1.9	1.6
ZPR6-7	*F28/F25*	1.7	6.3
	F49/F25	1.8	0.8
	C28/F25	1.0	1.5
ZPPR9	*F28/F25*	1.7	7.8
	F49/F25	1.8	0.9
	C28/F25	1.0	1.5
	Na Void Step 3	4.9	7.2
	Na Void Step 5	6.0	8.9
FLATTOP-Pu	*F28/F25*	2.1	1.9
	F37/F25	1.7	1.4
FLATTOP-25	*F28/F25*	2.1	1.9
	F49/F25	1.7	0.7
	F37/F25	1.4	1.6

Configuration	Integral parameter	APIA Simulation			
		1	2	1	2
		Covariance data			
		TENDL		COMMARA-2.0	
		A posteriori uncertainty (%)			
GODIVA	*F28/F25*	0.6	0.7	0.5	0.5
	F49/F25	0.3	0.3	0.2	0.2
	F37/F25	0.5	0.5	0.5	0.4
JEZEBEL-Pu239	*F28/F25*	0.5	0.4	0.2	0.3
	F49/F25	0.3	0.3	0.2	0.2
	F37/F25	0.4	0.5	0.3	0.3
ZPR6-7	*F28/F25*	0.5	0.6	1.0	0.8
	F49/F25	0.4	0.5	0.4	0.4
	C28/F25	0.4	0.4	0.7	0.6
ZPPR9	*F28/F25*	0.5	0.6	1.2	1.0
	F49/F25	0.4	0.5	0.4	0.4
	C28/F25	0.4	0.4	0.7	0.6
	Na Void Step 3	1.6	1.9	1.6	1.6
	Na Void Step 5	1.9	2.4	1.9	1.9
FLATTOP-Pu	*F28/F25*	0.5	0.5	0.3	0.3
	F37/F25	0.5	0.5	0.4	0.4
FLATTOP-25	*F28/F25*	0.5	0.6	0.6	0.5
	F49/F25	0.3	0.3	0.2	0.2
	F37/F25	0.4	0.5	0.5	0.5

A priori uncertainties (TENDL based cross-sections)

- Despite similarities , GODIVA and JEZEBEL-Pu239, *F28/F25* and *F37/F25*: individual contributions quite different.

GODIVA

F28/F25	TENDL cross-section	Uncertainty ≥ 0.5 (%)
TENDL covariances	^{238}U fission	1.4
	^{235}U fission	1.5
	^{235}U elastic	0.6
	^{235}U inelastic	1.2
COMMARA-2.0 covariances	^{238}U fission	0.5
	^{235}U inelastic	1.9
	^{235}U capture	0.8

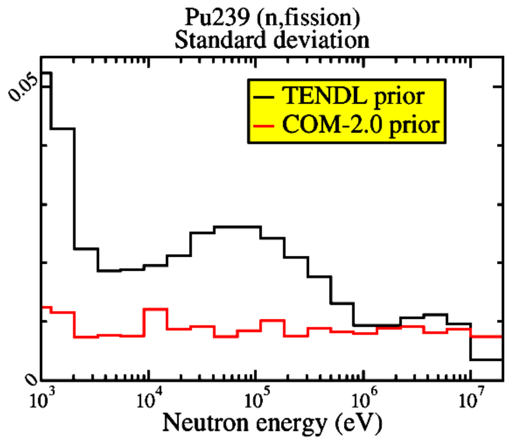
JEZEBEL-Pu239

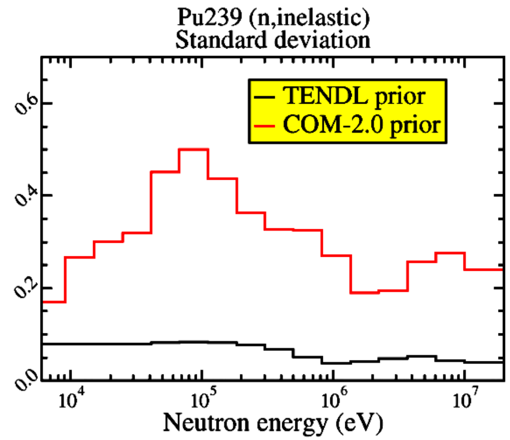
F28/F25	TENDL cross-section	Uncertainty ≥ 0.5 (%)
TENDL covariances	^{238}U fission	1.3
	^{235}U fission	1.9
	^{239}Pu inelastic	0.5
COMMARA-2.0 covariances	^{238}U fission	0.5
	^{239}Pu inelastic	2.4

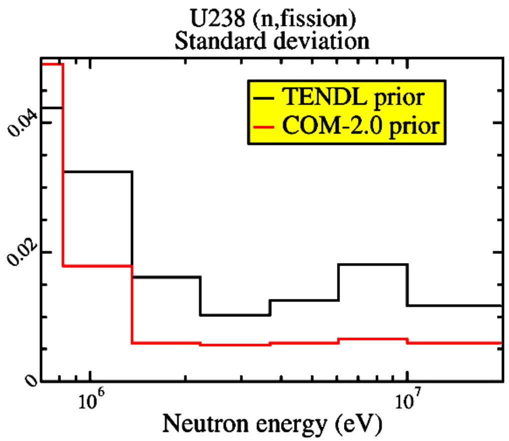
- TENDL: dominated by fission cross-section.
- COMMARA-2.0: dominated by inelastic scattering cross-section.

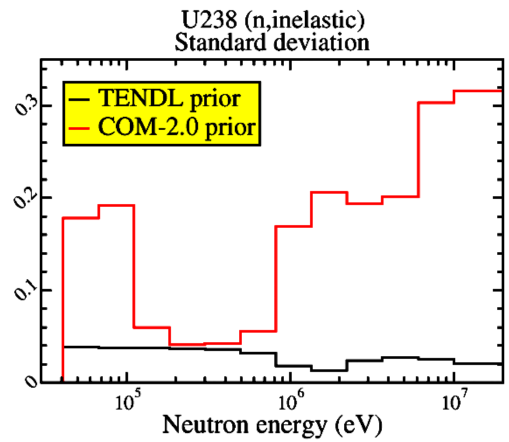
These compensations: consistent with covariance libraries (next figure).

Library standard deviations (TENDL versus COMMARA-2.0)









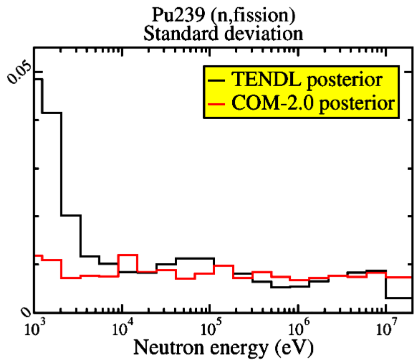
Different approach: model-based approach in TENDL tends limiting degree of freedom for inelastic scattering cross-section.

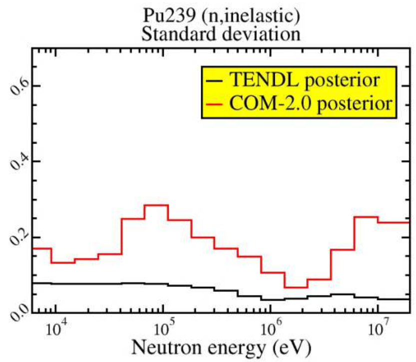
A posteriori uncertainties (TENDL based cross-sections)

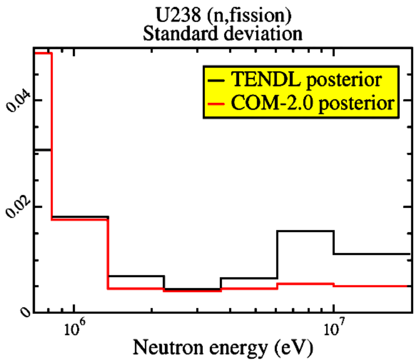
- Reduced as compared to a priori values.
- Do reflect C/E trends: largely simulation and covariance data independent.

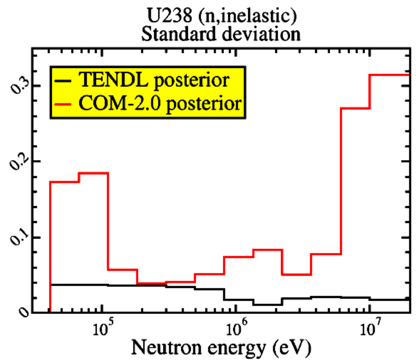
  Spectral indices: < experimental uncertainties.

  Coolant density effects: similar.





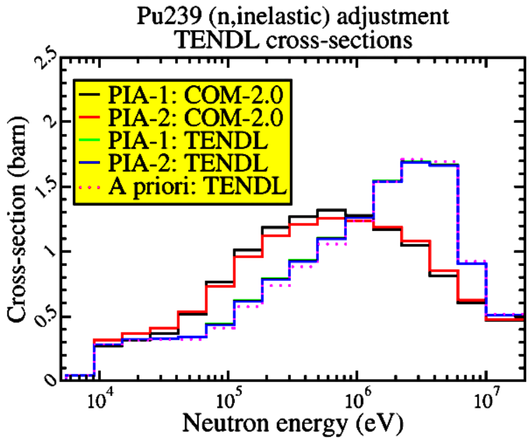




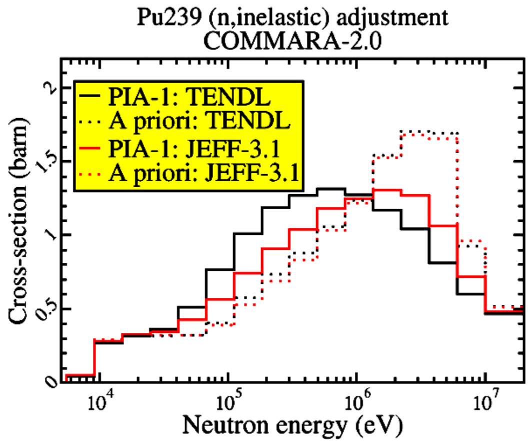
- Agreement between TENDL and COMMARA-2.0: assimilation, reduction of C/E uncertainties.

- Consistent with strong reductions of both TENDL fission cross-section and COMMARA-2.0 inelastic scattering cross-section.

A posteriori cross-sections: Pu239 inelastic



Same cross-sections, different covariances

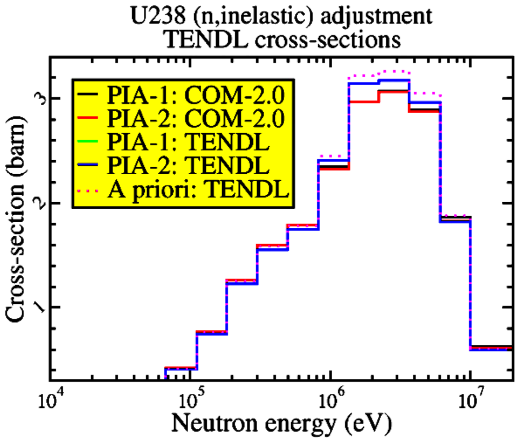


Same covariances, different cross-sections

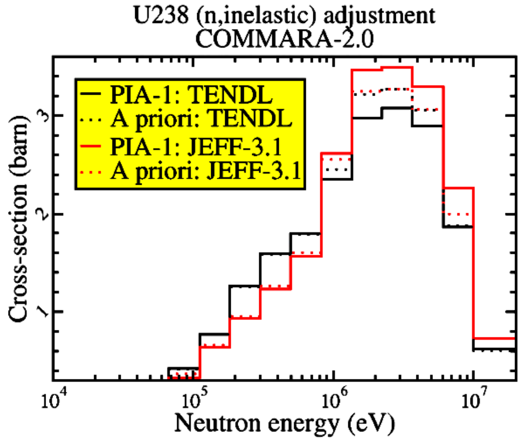
- A posteriori xs not unique.
- Adjustment of TENDL with COM-2.0:
  - ✓ much stronger since a priori standard deviations COM-2.0 > TENDL.
  - ✓ Not reliable: depends on APIA sequence.
- Adjustment of TENDL with TENDL:
  - ✓ Reliable, sequence independent.

- A posteriori xs not unique.
- Differences of a posteriori xs > Differences a priori xs.
- Adjustment trend similar between JEFF-3.1/COM-2.0 and TENDL/COM-2.0.

A posteriori cross-sections: U238 inelastic



Same cross-sections, different covariances

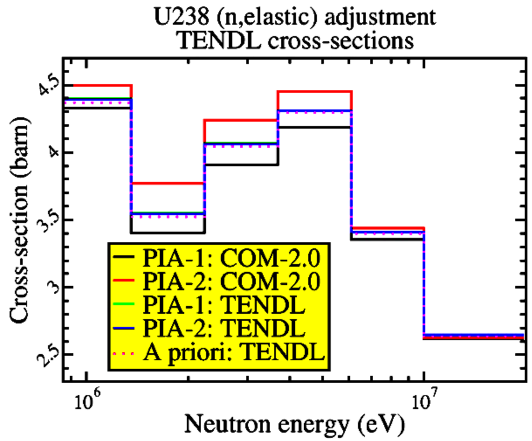


Same covariances, different cross-sections

- TENDL xs: to decrease mainly between 6.70MeV and 821keV (groups 3 -6); stronger decrease with COM-2.0.

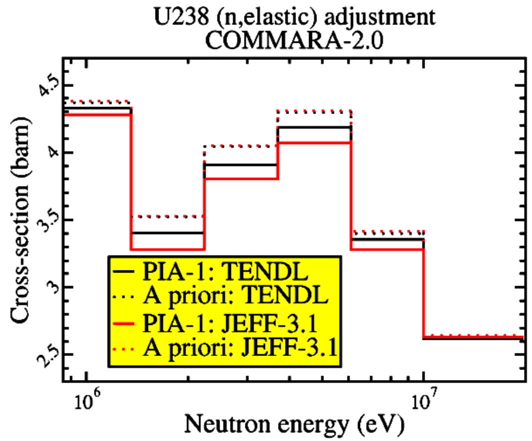
- Different adjustment trend between TENDL and JEFF-3.1.
- A posteriori JEFF-3.1 > A priori TENDL (contradiction, as also shown in previous study).

A posteriori cross-sections: U238 elastic



Same cross-sections, different covariances

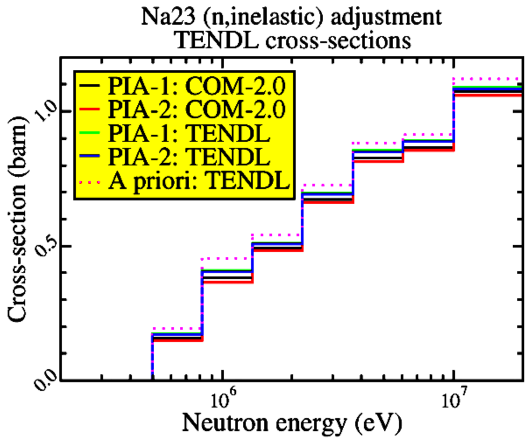
- Adjustment with COM-2.0: not appropriate.
- Weaker adjustment with TENDL: o.k.

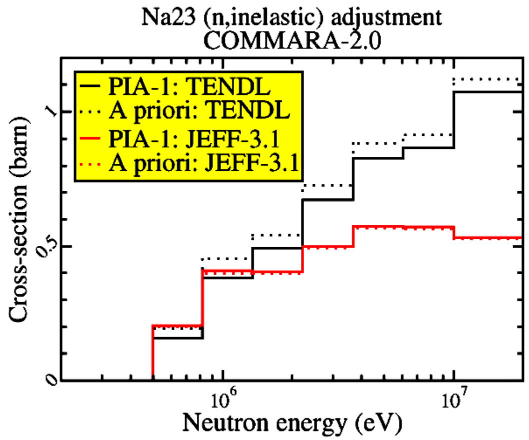


Same covariances, different cross-sections

- Different strength of adjustment, similar a priori cross-sections.

A posteriori cross-sections: Na23 inelastic





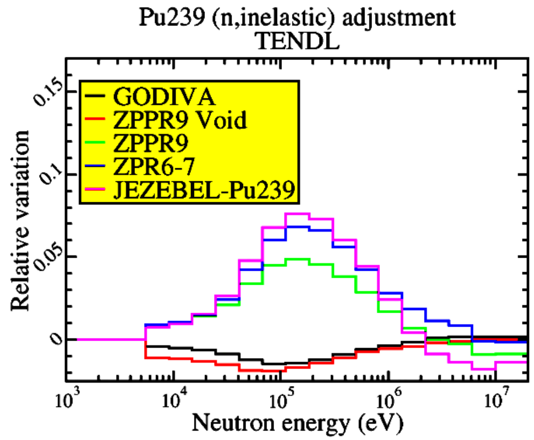
Same cross-sections, different covariances

- TENDL xs: to decrease.

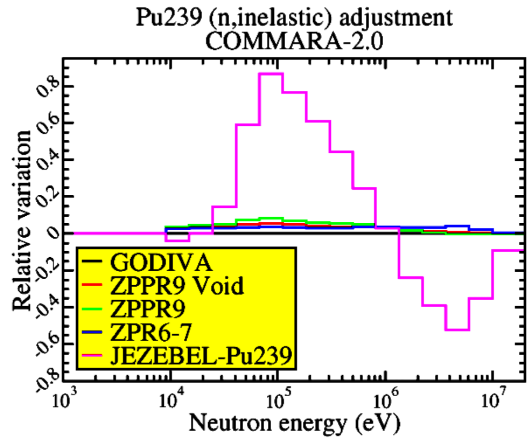
Same covariances, different cross-sections

- Large discrepancies between a priori TENDL and JEFF-3.1.
- Different adjustment trends reduce discrepancies but do not remove spread.

Incremental adjustment: Pu239 inelastic (APIA-1)



TENDL cross-sections; TENDL covariances

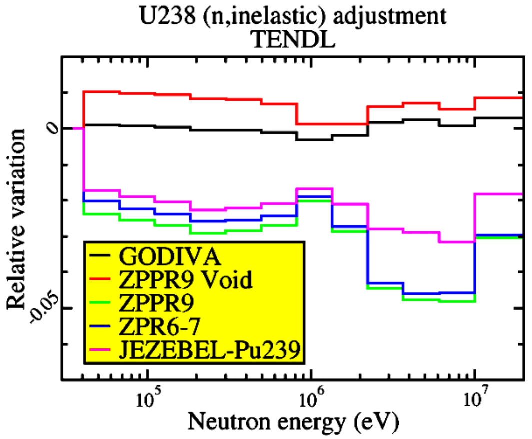


TENDL cross-sections; COMMARA-2.0 covariances

- Adjustment: primarily assimilation of ZPPR9 experimental data.

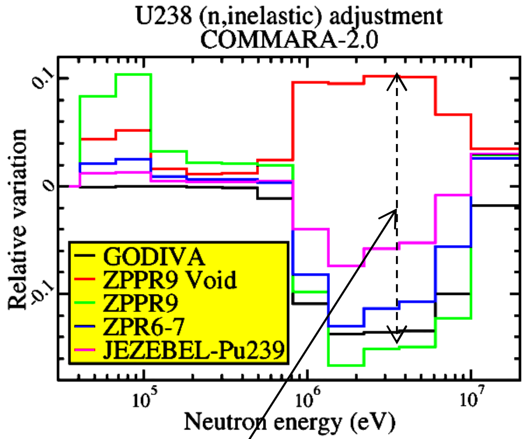
- Importance of individual steps depends on covariances. In this case ZPPR9 effect available, but assimilation of JEZEBEL-Pu239 much more important.

Incremental adjustment: U238 inelastic (APIA-1)



TENDL cross-sections; TENDL covariances

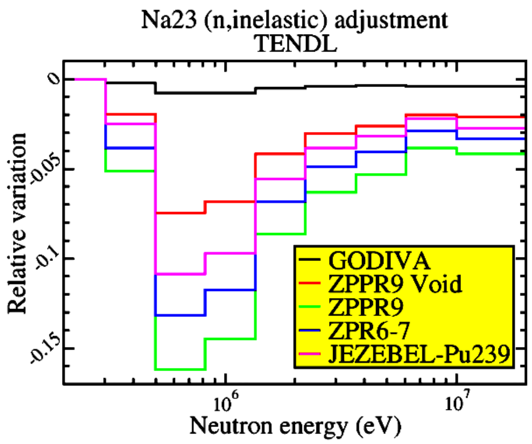
- Adjustment: primarily assimilation of ZPPR9 spectral indices.



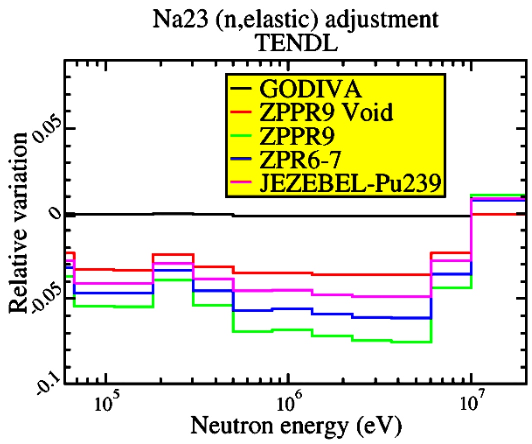
TENDL cross-sections; COMMARA-2.0 covariances

- Conflicts between steps e.g. between ZPPR9 coolant density and spectral indices assimilation.
- Consistent with APIA-1 ≠ APIA-2: adjustment not reliable.

Incremental adjustment: Na23 inelastic (APIA-1)



TENDL cross-sections; TENDL covariances



TENDL cross-sections; TENDL covariances

- Adjustment: primarily assimilation of ZPPR9 data.

Conclusions

- Differently from the other cases, the two APIA simulations using TENDL/TENDL i.e. consistent cross-sections and covariance data in terms of (1) data source, and (2) unified processing on the basis of the Total Monte Carlo method are able to provide similarly adjusted cross-sections by avoiding conflicting effects between incremental steps.
- These characteristics are indicative of reliable adjustments. Correspondingly it turns out that the TENDL inelastic scattering cross-sections of ^{238}U and ^{23}Na would need some reductions essentially due to the assimilation of ZPPR9 experimental data.

- **Key conclusion: reliable adjustments using the APIA methodology require full consistence between expectation values of the nuclear data and their covariances.**

Recommendations

- **Its is paramount understanding whether code specific adjustment trends of the *C/E*s are reproducible with a stochastic code and if the covariance data used to get the adjustment is sufficiently reliable.**

- Thus, consistently with statements of the original “Subgroup 39” mandate, “aiming to provide useful feedback to evaluators and differential measurement experimentalists in order to improve the knowledge of neutron cross sections to be used in a wider range of applications”

→ WPEC/SG-46, WPEC/SG-44.