Validating Pu-isotope ENDF/B-VIII.0 Nuclear Data with Critical Assemblies and Pulsed Spheres using Machine Learning Algorithms

CSEWG, Validation Session 12/2/20 Denise Neudecker

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How did we validate Pu-isotope (²³⁸⁻²⁴²Pu) nuclear data?

<u>Statistics tools used</u>: Random forests and SHAP metric. Shown to be able to highlight issues in nuclear data in Neudecker et al., NDS 167, 36-60 (2020).

Nuclear data validated: ²³⁸⁻²⁴²Pu for ENDF/B-VII.1 and ENDF/B-VIII.0.

Validation experiments used:

- 875 criticality experiments
- 15 LLNL pulsed-sphere neutron-leakage spectra

Additional information used for validation:

- Systematic comparison of nuclear data with differential experimental data from EXFOR (only in rare cases detailed analysis)
- Nuclear-theory considerations







Validation of ²⁴¹Pu nuclear data: this is a challenge due to compensating errors!

Energy ranges and observables highlighted as problematic by ML.

Energy (MeV)	PFNS	Nu-bar	(n,f)	(n,g)	(n,el)	(n,inl)
Thermal						
7e-8-1e-5						
1-5.5e ⁻⁴						
5.5e ⁻⁴ -2.5e ⁻²						
2.5e ⁻² -2.479						
2.479-4.8						
4.8-8.187						

No Diff. Exp.



Exp. Agree with evaluation but freedom to move

Diff. Exp. Disagree with evaluation



"Highlights" of issues in ²⁴¹Pu nuclear data:

Can we extend resonance range of (n,f), (n,el) and (n,g)?



High-level summary of issues in ²⁴¹Pu nuclear data:

Issues that are recommended to be investigated for a new release:	 (n,f) cross section from 0.1-2 MeV. Replace PFNS with an evaluation that captures the physics expected behavior better. Investigate if it is possible to extend the resonance range to higher E_{inc}.
Potential freedom in nuclear data that could be exploited to obtain better agreement with validation experiments:	 Get a finer grid for nu-bar. Investigate if it is feasible and beneficial to get closer to some standards at thermal, especially (n,f) and nubar (the (n,f) thermal value differs by about 1 sigma from standard value).



Validation of ²³⁹Pu nuclear data: also a challenge due to compensating errors!

Energy ranges and observables highlighted as problematic by ML.

Energy (MeV)	PFNS	Nu-bar	(n,f)	(n,g)	(n,el)	(n,inl)	(n,2n)
Thermal							
5e ⁻⁸ -4e ⁻⁷							
4e ⁻⁷ -8.1e ⁻⁶							
8.1e ⁻⁶ -0.1							
0.1-2.354							
2.354-8.187							

No Diff. Exp.



Exp. Agree with evaluation but freedom to move

Diff. Exp. Disagree with evaluation



High-level summary of issues in ²³⁹Pu:

Issues that are recommend ed to be investigated for a new release:	 Re-evaluate PFNS with recent Chi-Nu and CEA exp. data. (n,f): Are there structures in the URR? (see Bertsch, PRC 98, 014611 (2018)); where should the eval. cs above 10 MeV go? 	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
Potential freedom in nuclear data that could be exploited to obtain better agreement with validation experiments:	 After PFNS is fixed, one might investigate thermal constants compared to standard values. Incorporate newest (n,f) standard. 0.3-17 keV for nu-bar (no exp. data) and tweaking nu-bar in the fast. Balance (n,tot), (n,el) & (n,inl) cs from 0.1-2.4 MeV. 	0.1 1 Outgoing Neutron Energy (MeV)	10 10 10 10 10
		VIII.0 at 13.75 Me	эV



Slide 7

Validation of ²⁴⁰Pu nuclear data:

Energy ranges and observables highlighted as problematic by ML.

Energy (MeV)	PFNS	Nu-bar	(n,f)	(n,g)	(n,el)	(n,inl)
Thermal						
3.25e-7-5.5e-4						
5.5e-4-2.5e-2						
2.5e ⁻² -1.85						
1.85-3						
3-12.84						
12.84-15.68						



No Diff. Exp.

Exp. Agree with evaluation but freedom to move

Diff. Exp. Disagree with evaluation



Slide 8

High-level summary of issues in ²⁴⁰Pu:

Issues that could be investigate d:	 Is the shape of nu-bar physical? (0.5-0.9, 4-6, 13-15 MeV) Study (n,f) cs in the fast range 	94-Pu-240(H, F)PR, HU 6 Prompt nu-bar 5
Potential freedom in nuclear data:	 Re-evaluate PFNS with Chi-Nu exp. if different (avoid compensating effects) Is there an issue in the (n,el) cs from 0.9-1.2 MeV? Exp. Data might be misleading. 	A A A A A A A A A A A A A A A A A A A





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Cross Section (barns)

Validation of ²³⁸Pu nuclear data:

Energy ranges and observables highlighted as problematic by ML.

Energy (MeV)	PFNS	Nu-bar	(n,f)	(n,g)	(n,el)	(n,inl)
Thermal						
1e ⁻⁷ -3.25e ⁻⁷						
3.25e ⁻⁷ -8.1e ⁻⁶						
8.1e ⁻⁶ -1.7e ⁻²						
1.7e ⁻² -0.9						
0.9-2.479						
2.479-3						



No Diff. Exp.

Exp. Agree with evaluation but freedom to move

Diff. Exp. Disagree with evaluation





High-level summary of issues in ²³⁸Pu:

5×10⁻⁸

2×10-9

5×10-9

10⁻⁸ 2×10⁻⁸

Incident Energy (MeV)

10-7

2×10-7

Issues that could be investigate d:	 Re-evaluate thermal nu-bar using exp. data (n,g): study exp. Data close to ~1e⁻⁷ and for 1e⁻⁵-1e⁻³ MeV 	³ (<i>n</i> , <i>f</i>) cross sections			
Potential freedom in nuclear data:	 (n,f): check at thermal, one can tweak from 0.1–3 MeV. 	$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\$			
2×10 ⁻⁹ 5×10 ⁻⁹ 2×10 ³ 10 ³ 5×10 ² 2×10 ² 10 ² 50 (<i>n,g</i>) 0	10 ⁻⁸ 2*10 ⁻⁸ 5*10 ⁻⁸ 10 ⁻⁷ 2*10 ⁻⁷ 2*10 ³ 10 ³ 10 ³ 5*10 ² 10 ² 10 ² 5 ⁵ 10 ² 10 ³ 10 ² 10 ³ 10 ² 10 ³ 10 ² 10 ³ 10 ² 10 ³ 10 ³ 10 ² 10 ³ 10 ³ 10 ² 10 ³ 10 ² 10 ³ 10 ² 10 ³ 10 ³ 10 ² 10 ²	$5 \times 10^{-6} 10^{-5} 5 \times 10^{-5} 10^{-4} 5 \times 10^{-4} 10^{-3} 10^{-3} 10^{-4} 10^{-3} $			

5×10⁻⁶ 10⁻⁵

10-4

5×10⁻⁵ Incident Energy (MeV) 5×10⁻⁴ 10⁻³

Validation of ²⁴²Pu nuclear data:

Energy ranges and observables highlighted as problematic by ML.

Energy (MeV)	PFNS	Nu-bar	(n,f)	(n,g)	(n,el)	(n,inl)
Thermal						
1.5e ⁻⁷ -2e ⁻⁷						
2e ⁻⁷ -3e ⁻⁶						
3e ⁻⁶ -3e ⁻³						
3e ⁻³ -1.72e ⁻²						
1.72e ⁻² -0.9						
0.9-6.434						

No Diff. Exp.

Exp. Agree with evaluation but freedom to move

Diff. Exp. Disagree with evaluation





High-level summary of issues in ²⁴²Pu:



Summary

- We validated ²³⁸⁻²⁴²Pu ENDF/B-VIII.0 nuclear data with respect to 875 critical assemblies and 15 pulsed spheres. We also compared evaluated data to differential data from EXFOR and took into account basic theoretical considerations.
- CAVEAT: experimental data were not analyzed in detail and a comparison to EXFOR as is might be misleading. SG-50 might help for such undertakings.
- A (down-selected) listing of potential issues in nuclear data that could be investigated for a new release was shown.
- Some hints potential freedom to move nuclear data is given.
- Is someone interested in helping us investigate resonance-range issues?



Thank you for your attention!



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