Evaluations for $^{235,238}$U and $^{239}$Pu fission-source term observables

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This work shows progress towards fulfilling NCSP milestones of LANL ND1 (Nuclear Data Evaluation and Testing).

FY22-23 milestones:

- $^{235}\text{U}$, $^{239}\text{Pu}$: “Evaluate PFNS and multiplicity consistently, including angular information about prompt neutrons” (FY22 Q4),
- $^{235}\text{U}$: “Develop consistent evaluation of fission yields, neutron multiplicity, and spectra from thermal to 20 MeV” (FY22 Q4)
- $^{238}\text{U}$: “Evaluate PFNS and multiplicity consistently, including angular information about prompt neutrons” (FY22 Q4),
- $^{235}\text{U}$: “Finalize prompt fission neutron spectra based on LANSCE high-energy emission data from Chi-Nu” (FY22 Q2),
- $^{238}\text{U}$: “Finalize prompt fission neutron spectra based on LANSCE Chi-Nu Data” (FY23 Q4),
- $^{238,240-242}\text{Pu}$: “Attempt a consistent nu-bar evaluation supported by a model code to provide better evaluated nu-bar for minor Pu-isotopes” (FY23 Q4).
FY22-23 milestones:

- $^{235}$U, $^{239}$Pu: “Evaluate PFNS and multiplicity consistently, including angular information about prompt neutrons” (FY22 Q4),
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- $^{238}$U: “Finalize prompt fission neutron spectra based on LANSCE Chi-Nu Data” (FY23 Q4),
- $^{238,240-242}$Pu: “Attempt a consistent nu-bar evaluation supported by a model code to provide better evaluated nu-bar for minor Pu-isotopes” (FY23 Q4).

Four milestones are reached with the LANL-developed Hauser-Feshbach Fission Fragment Decay Codes CGMF (Monte Carlo) and BeoH (deterministic)
Modeling and related milestones

- **Milestone: $^{235}\text{U}$:** “Develop consistent evaluation of fission yields, neutron multiplicity, and spectra from thermal to 20 MeV” (FY22 Q4)
  - Lovell, Kawano, et al., *PRC* 103 014615 (2021)
- **Milestone: $^{238,240-242}\text{Pu}$:** “Attempt a consistent nu-bar evaluation supported by a model code to provide better evaluated nu-bar for minor Pu-isotopes” (FY23 Q4).
  - Lovell and Neudecker, LA-UR-22-29570
Monte Carlo and deterministic models at LANL

Input needed from theory and experiment:

• First-principle calculations of fission yields
• Multi-chance fission probabilities
• Pre-fission neutron energy spectra
• Mass, charge, and kinetic energy of fission yields

Monte Carlo: CGMF (prompt)

Deterministic: BeoH (prompt and delayed)
Average neutron multiplicities and fission product yields can be reproduced simultaneously (BeoH)

Consistency among Pu isotopes is being developed (CGMF, towards FY23 milestone)

$^{239}\text{Pu}(n,f)$ and $^{241}\text{Pu}(n,f)$ are already included in CGMF. The parametrizations can be interpolated to calculate $^{240}\text{Pu}(n,f)$. First results – without any optimization – are promising.

Lovell and Neudecker, LA-UR-22-29570

TKE and neutron multiplicity already agree reasonably well with experimental data
Evaluation and related milestones

• Milestone: \(^{235}\text{U}, \, ^{239}\text{Pu}\): “Evaluate PFNS and multiplicity consistently, including angular information about prompt neutrons” (FY22 Q4):
  - \(^{239}\text{Pu}\) nu-bar, PFNS and \((n,f)\) cross section: Neudecker, Lovell et al., Frontiers in Physics Vol. 10, (2022); https://doi.org/10.3389/fphy.2022.1056324
  - \(^{235}\text{U}\) nu-bar: Lovell, Neudecker, Talou, LA-UR-22-23475

• Milestone: \(^{238}\text{U}\): “Evaluate PFNS and multiplicity consistently, including angular information about prompt neutrons” (FY22 Q4):
  - Neudecker, Lovell, Kawano and Talou, LA-UR-22-29906
We get evaluated data and covariances with GLLS using model data as a prior and updating with exp. info.

GLLS combines:

- Model ("M") mean values and covariances,
- Experimental mean values ("x") and covariances,
- To evaluated mean values and covariances ("post") for a ND file using,
- The design matrix S that either transforms from model parameter space to observable space or from energy lattice of the model to exp. one.

$$\phi_{\text{post}} = \phi^M + \text{Cov}^\text{post} S^+ (\text{Cov}^x)^{-1} (\phi^x - S\phi^M) ,$$

$$\text{Cov}^\text{post} = \text{Cov}^M - \text{Cov}^M S^+ (S\text{Cov}^M S^+ + \text{Cov}^x)^{-1} S\text{Cov}^M$$

As prior, we either use information from CGMF or Los Alamos model.
We produced for the first time ENDF/B-quality nu-bar using CGMF. *Eval.* $^{239}$Pu nu-bar and cov in VIII.1β1.

**Difference to ENDF/B-VIII.0:**
(a) New high-precision data by Marini (CEA) using Chi-Nu array,
(b) improved UQ of past experimental data (template of expected exp. unc.),
(c) using CGMF modeling consistent with TKE, FY, etc.

New compared to TPR 2022: covariances supplied.
The eval. parameters of $^{239}\text{Pu}(n,f)$ nu-bar produce realistic estimates of fission quantities with CGMF.

The only problem is that the PFNS is predicted too soft.
We produced also ENDF/B-quality $^{235}$U nu-bar using CGMF. Eval. $^{235}$U nu-bar and cov in VIII.1β1.

**Difference to ENDF/B-VIII.0:**

a) Included 2 new data sets (Boikov, Khoklov),

b) Improved UQ of past experimental data (template of expected exp. unc.),

c) Using CGMF modeling consistent with TKE, Y(A), etc.

New compared to TPR 2022: data finalized & accepted, covariances supplied.
The evaluated parameters link favorably back to other fission quantities, except for PFNS, using CGMF.

Using CGMF for evaluations brings the added benefit that we can link back nu-bar to Y(A), TKE(A), etc. to see if they are all consistent and realistic.
Evaluated $^{238}\text{U}$ nu-bar, with and without CGMF, differs from ENDF/B-VIII.0 from 2-4 MeV. New experimental data needed.

Need to counter-balance change in nu-bar by PFNS. Chi-Nu delivered FY23 data. nu-bar to be measured by CEA.

ENDF/B-VIII.0:

a) VIII.0 based on Frehaut, no detailed UQ of past data,

b) No model!
The evaluated parameters link favorably back to other fission quantities, except for PFNS, using CGMF.

We are doing reasonably fine in describing $Y(A)$, but $<\text{TKE}>$ not as well-described (large spread in data). New experimental nu-bar will help.
Evaluation

• Milestone: $^{235}$U: “Finalize prompt fission neutron spectra based on LANSCE high-energy emission data from Chi-Nu” -> we did that also for $^{239}$Pu

• Milestone: $^{238}$U: “Finalize prompt fission neutron spectra based on LANSCE Chi-Nu Data” (FY23 Q4)
  - Keegan Kelly delivered data for evaluation to Denise Neudecker December 2022,
  - modeling, exp. UQ, and evaluation ongoing.
Eval. $^{239}$Pu PFNS and cov using Chi-Nu & CEA data and Los Alamos model are in VIII.1β1.

(a) Difference to VIII.0: High-precision Chi-Nu & CEA PFNS,
(b) Same as VIII.0: Los Alamos model (DN et al., NDS 148, 293 (2018)).

Mean energy uncertainty at $E_{\text{inc}} = 1.5$ MeV: 33.7 keV.

New compared to TPR 2022: covariances supplied.
Eval. $^{235}\text{U}$ PFNS and covariance using Chi-Nu data and Los Alamos model are in VIII.1β1.

(a) Difference to VIII.0: All high-precision Chi-Nu PFNS,
(b) Same as VIII.0: Los Alamos model (DN et al., NDS 148, 293 (2018)).

Mean energy uncertainty at $E_{\text{inc}} = 1.5$ MeV: 28 keV.

New compared to TPR 2022: PFNS finalized, data accepted, covariances supplied, benchmarking done.
Ratio of VIII.1 $\beta_1$ $^{239}\text{Pu}/^{235}\text{U}(n,f)$ PFNS at $E_{\text{inc}} = 1.5$ MeV remains in good agreement with experimental data.

![Graph showing comparison between calculated and experimental data for $^{239}\text{Pu}/^{235}\text{U}$ PFNS at $E_{\text{inc}} = 1.5$ MeV.](image)
New evaluated $^{235}$U nu-bar and PFNS lead to small changes in $k_{\text{eff}}$ of a few HEU and IEU MET-FAST experiments.

Table II: Simulated and experimental $k_{\text{eff}}$ values are compared with each other for ENDF/B-VIII.0, ENDF/B-VIII.0 with the new PFNS for $E_{\text{inc}}=0.5$–30 MeV and ENDF/B-VIII.0 with the new PFNS for $E_{\text{inc}}=0.5$–30 MeV and a tweaked $\bar{\nu}_p$ from Refs. [27, 28]. An abbreviated ICSBEP nomenclature is used to identify the ICSBEP critical assembly [7]. HMF001 is the Godiva assembly, HMF028 is Flattop, IMF1 is Jemima and IMF7 is BigTen.

<table>
<thead>
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<th>Benchmark</th>
<th>Exp.</th>
<th>Exp. Unc. (pcm)</th>
<th>VIII.0</th>
<th>PFNS</th>
<th>PFNS-VIII.0 (pcm)</th>
<th>$\bar{\nu}$+PFNS</th>
<th>$(\bar{\nu}$+PFNS)-VIII.0 (pcm)</th>
<th>MC Unc. (pcm)</th>
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<td>1.00421</td>
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</table>
New evaluated $^{235}$U PFNS improves simulated neutron leakage spectra of LLNL pulsed spheres.

New integral exp. mapping out the $^{235}$U PFNS are coming, and will be used for validation.
Summary

• Currently in VIII.1β1:
  – $^{239}$Pu nu-bar including CGMF modeling and CEA data,
  – $^{239}$Pu PFNS including Chi-Nu & CEA data,
  – $^{239}$Pu$(n,f)$ cross section including fissionTPC data.
  – $^{235}$U nu-bar including CGMF modeling,
  – $^{235}$U PFNS including Chi-Nu data.

• Delivered:
  – $^{238}$U nubar including CGMF modeling,
  – $^{238}$U Chi-Nu PFNS.

To-Do:
• Model, exp. UQ, and evaluate $^{238}$U PFNS including at higher $E_{\text{inc}}$,
• Benchmark $^{238}$U PFNS & nu-bar evaluations,
• Get $^{238,240-242}$Pu nu-bar.

Thank you for your attention!

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Back-up

- Modeling
- Experimental UQ
Initial conditions of the fission fragments are modeled phenomenologically, fit to available experimental data.

These initial conditions are essentially shared between the two codes – we can utilize optimization from one code for the other.

\[ \rho(J) = \frac{1}{2} (2J + 1) \exp \left[ -\frac{J(J + 1)}{2B^2} \right] \]

\[ B^2 = \alpha \frac{I_0(A, Z)T}{\hbar^2} \]

\[ Y(A, Z, TKE, J, \pi) \]
The Hauser-Feshbach statistical theory is used to de-excite the fission fragments

Other nuclear information is needed for modeling
• Discrete nuclear levels (RIPL)
• Optical model potential (e.g. Koning Delaroche)
• Level densities
• Nuclear masses

Many models are constrained by experimental data, which is plentiful closer to the stable nuclei – not the case for the excited nuclei that are created during the fission process

Energy, momentum, spin, and parity are conserved during the decay
Historically, the PFNS has been a challenge to reproduce with any Hauser-Feshbach decay model. Changes to the fission fragment initial conditions that stay within the bounds of other observables (e.g. Y(A), TKE, multiplicities) can only move the PFNS so far.

LA-UR-21-30882

PFNS evaluations are still performed using the Los Alamos Model while further studies are ongoing.
Exp. database & covariances are obtained with the code ARIADNE

ARIADNE modules:
• PFNS exp. UQ,
• Nu-bar exp. UQ,
• (n,f) cross section UQ,
• Evaluations (Kalman, GLLS),
• Creating databases for evaluations in json, txt, previously xml.

UQ done:
• Implements templates of exp. unc. & unc./ metadata from EXFOR.
• A python notebook exists for each exp.

238U nu-bar exp. cov. estimated with ARIADNE.