EFF/DOC-1144
A Comparison of different Uncertainty Activation Cross-Section Data Libraries:
Application to the Prediction Uncertainty in Tritium Production

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INTRODUCTION. The context of this work …

- EFFDOC – 1113: “Measurements of tritium activity in HCLL TBM mock-up LiPb material irradiated in the Frascati experiment” (by W. W. Pohorecki) JEFF/EFF Meeting Paris, 31 May-2 June 2010

- T activity in LiPb mock-up material irradiated in Frascati: measurement and MCNP results.

Figure 1: Slit 1-8, $^3$H activity in LiPb
INTRODUCTION. The context of this work …

- EFFDOC – 1135: “Analysis of the HCLL Blanket Mock-up Experiment” (by R. Villari et al.) JEFF/EFF Meeting Paris, [This meeting]

Uncertainties on TPR determination

- Proposed definitive uncertainty on C/E comparison

  ✓ experimental errors (Li-6) 3.7%
  ✓ uncertainty on FNG source intensity 3%
  ✓ Monte Carlo calculation statistics < 1%
  ✓ cross sections < 2%
  ✓ Pb-Li composition 1%*

\[ \Delta (C/E) \sim 5.3 \% \ (1\sigma) \]

- As a general result C/E are close to one within the total combined uncertainties (~±10% at 2\sigma level)

*Sensitivity of TPR to Li6 content : -0.5%/%
Error propagation techniques for activation

Goal: “to analyse how ND uncertainty is transmitted to N”

\[
\frac{d}{dt} N = AN
\]

\[N = (N_1, N_2, \ldots)\]
\[\sigma = (\sigma_1, \sigma_2, \ldots)\]

\[\Rightarrow N_i = N_i(\sigma)\]

1) Sensitivity / Uncertainty Analysis (S/U)

- Method based on the first order Taylor series to estimate uncertainty indices for each reaction cross section in a continuous irradiation scenario *(linear approximation)*

2) Monte Carlo Uncertainty Analysis (MC)

- To treat the global effect of all cross sections uncertainties in activation calculations, we have proposed an uncertainty analysis methodology based on Monte Carlo random sampling of the cross sections

- Assignment of a Probability Density Function (PDF) to each cross section
1. Sensitivity/Uncertainty Analysis

We assume:

\[ N_i = N_i(\sigma, \phi, \text{fission yields}, \phi(E), N_0) \implies N_i(\sigma) \approx N_i(\sigma_0) + \sum_{j=1}^{m} \frac{\partial N_i}{\partial \sigma_j} \frac{\sigma_j - \sigma_{j0}}{\sigma_{j0}} \]

Relative error in \( N_i \) due to changes in cross-sections:

\[ e_i = \rho_{i1} \varepsilon_1 + \rho_{i2} \varepsilon_2 + \cdots + \rho_{im} \varepsilon_m \]

Cross-section sensitivity coefficient (FSAP, ASAP, …)

\[ \| e_i \| = \rho_{i1}^2 \Delta_1^2 + \rho_{i2}^2 \Delta_2^2 + \cdots + \rho_{im}^2 \Delta_m^2 \]

\[ \text{Var}(e_i) = \rho_i^T V \rho_i \]

Information obtained processing ND

\[ \text{Var}(\varepsilon) = V \]

(sandwich formula)
2. Monte Carlo method

- We use simultaneous random sampling of all the XS PDFs involved in the problem. PDF is assigned to each $\sigma_j$: $\sigma_j \rightarrow N(\sigma_{j0}, \text{var}(\sigma_j)) \quad \Rightarrow \quad \varepsilon_j \rightarrow N(0, \Delta^2_j)$

  $\Rightarrow$ For large values of $\Delta_j$, $\sigma_j$ could be negative!

- PDF assumed to be lognormal: $\log(\sigma_j / \sigma_{j0}) = \log(1 + \varepsilon_j) \approx \varepsilon_j \rightarrow N(0, \Delta^2_j)$

From the sample of the random vector $\sigma$, $\sigma = (\sigma_1, \ldots, \sigma_j, \ldots, \sigma_m)$ the matrix $A$ is computed and the vector of nuclide quantities $X$ is obtained $N = (N_1, \ldots, N_i, \ldots, N_n)$

Repeating the sequence, we obtain a sample of isotopic concentration vectors. The statistic estimators of the sample can be estimated

Enables to investigate the global effect of the complete set of $\Delta\sigma$ on $N$
### Figure 2: Tritium Uncertainty Prediction in SL1 and SL7 using EAF2007/UN

<table>
<thead>
<tr>
<th></th>
<th>SL1: Natural Abundance</th>
<th>SL1: Depleted Li6</th>
<th>SL7: Natural Abundance</th>
<th>SL7: Depleted Li6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Bq (at shutdown)</td>
<td>7.25% Li6 in Li</td>
<td>3.92</td>
<td>3.47</td>
<td>0.64</td>
</tr>
<tr>
<td>Only due to Li</td>
<td>3.78</td>
<td>3.33</td>
<td>0.64</td>
<td>0.28</td>
</tr>
<tr>
<td>Only Li6</td>
<td>0.96</td>
<td>0.40</td>
<td>0.62</td>
<td>0.26</td>
</tr>
<tr>
<td>Only Li7</td>
<td>2.82</td>
<td>2.93</td>
<td>0.02</td>
<td>0.02</td>
</tr>
</tbody>
</table>

#### Sensitivity Coefficient: \( \rho = \frac{(DN/N)}{(DXS/XS)} \) in %

<table>
<thead>
<tr>
<th></th>
<th>SL1</th>
<th>SL7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li6(n,T)He4</td>
<td>0.25</td>
<td>0.12</td>
</tr>
<tr>
<td>Li7(n,na)T</td>
<td>0.72</td>
<td>0.84</td>
</tr>
<tr>
<td>F19(n,T)</td>
<td>0.04</td>
<td>1.14E-06</td>
</tr>
<tr>
<td>Mg25(n,T)</td>
<td>...</td>
<td>6.36E-03</td>
</tr>
</tbody>
</table>

#### Sensitivity/Uncertainty (%): \( \rho \Delta \)

<table>
<thead>
<tr>
<th></th>
<th>SL1</th>
<th>SL7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li6(n,T)He4</td>
<td>0.82</td>
<td>0.38</td>
</tr>
<tr>
<td>Li7(n,na)T</td>
<td>47.83</td>
<td>56.21</td>
</tr>
<tr>
<td>F19(n,T)</td>
<td>0.70</td>
<td>...</td>
</tr>
</tbody>
</table>

#### Uncertainty with Monte Carlo

<table>
<thead>
<tr>
<th></th>
<th>SL1</th>
<th>SL7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean value</td>
<td>4.67</td>
<td>4.27</td>
</tr>
<tr>
<td>Relative error (%)</td>
<td>58.62</td>
<td>67.03</td>
</tr>
</tbody>
</table>

- \( \rho \): is the sensitivity coefficient for the tritium production
- \( \Delta \): is the corresponding relative error collapsed in 1 group
- the index “\( \rho \Delta \)” that can be used to rank cross sections inducing the highest uncertainties
To take into account …: Linear Perturbation Theory

Applicability of 1st Taylor-series expansion

The deterministic approach should be used wherever it provides sufficiently accurate results. Normally, this will be the case when errors are relatively small and the conditions not extreme.
To take into account …: Monte Carlo sampling

Mean Value: $T_M = 4.27$ Bq/g; and relative error: 67.03%

It fits to a logNormal distribution

Min: 0.93
Max: 31.57
$^7$Li(n,T) – EAF 2010&2007 Uncertainties

Incident neutron data // Li7 //

EAF2007: Relative Error ~66%
EAF2010: Relative Error ~33%
EAF2007-PENDF
EAF2010-VITJ175
\( ^7\text{Li}(n,T) – \text{EAF 2010}&2007: \text{Covariance matrix} \)

- Given \( \mathbf{V} \) the G-by-G variance matrix of the relative XSs vector, the variance \( \Delta^2 \) of the relative spectrum-averaged cross section is:
  \[
  \Delta^2 = \mathbf{\omega}^T \mathbf{V} \mathbf{\omega}
  \]
  with \( \mathbf{\omega} = \left[ \frac{1}{\phi} \, \frac{\sigma_1}{\sigma^{\text{eff}}} , \ldots , \frac{\phi_G}{\phi} \, \frac{\sigma_G}{\sigma^{\text{eff}}} \right]^T \)

- Assuming \( \Delta^2_{\text{I=1,EAF}} \) (relative error, \( \Delta \))
  \[
  \rightarrow \Delta_{\text{I=1,EXP}} = \frac{\Delta_{\text{I=1,EAF}}}{3}
  \]

### Uncert_1group (EAF2007) = \( \Delta \)

<table>
<thead>
<tr>
<th>Reaction</th>
<th>( \Delta^2_{\text{EAF2007}} )</th>
<th>Relative Exp Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li6(n,T)He4</td>
<td>0.01</td>
<td>3.33</td>
</tr>
<tr>
<td>Li7(n,na)T</td>
<td>4.00</td>
<td>66.67</td>
</tr>
<tr>
<td>F19(n,T)</td>
<td>0.36</td>
<td>20.00</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F19(n,nT)</td>
<td>16.00</td>
<td>133.33</td>
</tr>
</tbody>
</table>

### Uncert_1group (EAF2010) = \( \Delta \)

<table>
<thead>
<tr>
<th>Reaction</th>
<th>( \Delta^2_{\text{EAF2010}} )</th>
<th>Relative Exp Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li6(n,T)He4</td>
<td>0.01</td>
<td>3.33</td>
</tr>
<tr>
<td>Li7(n,na)T</td>
<td>1.00</td>
<td>33.33</td>
</tr>
<tr>
<td>F19(n,T)</td>
<td>0.36</td>
<td>20.00</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F19(n,nT)</td>
<td>4.00</td>
<td>66.67</td>
</tr>
</tbody>
</table>
$^7\text{Li}(n,T)$ - ENDF/B-VII vs EAF2010

EAF2010: Relative Error \(~33\%\)

Tritium production is not in one MT number:
MT853+MT854+MT855+ \ldots = (n,n'at)
$^7\text{Li}(n,T)$ - ENDF/B-VII: Covariance Matrix in 44g

Ordinate scales are % relative standard deviation and barns.
Abscissa scales are energy (eV).

Correlation Matrix

<table>
<thead>
<tr>
<th></th>
<th>1.0</th>
<th>0.8</th>
<th>0.6</th>
<th>0.4</th>
<th>0.2</th>
<th>0.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>0.8</td>
<td>0.6</td>
<td>0.4</td>
<td>0.2</td>
<td>0.0</td>
</tr>
<tr>
<td>0.8</td>
<td>0.8</td>
<td>1.0</td>
<td>0.8</td>
<td>0.6</td>
<td>0.4</td>
<td>0.2</td>
</tr>
<tr>
<td>0.6</td>
<td>0.6</td>
<td>0.8</td>
<td>1.0</td>
<td>0.8</td>
<td>0.6</td>
<td>0.4</td>
</tr>
<tr>
<td>0.4</td>
<td>0.4</td>
<td>0.6</td>
<td>0.8</td>
<td>1.0</td>
<td>0.8</td>
<td>0.6</td>
</tr>
<tr>
<td>0.2</td>
<td>0.2</td>
<td>0.4</td>
<td>0.6</td>
<td>0.8</td>
<td>1.0</td>
<td>0.8</td>
</tr>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.2</td>
<td>0.4</td>
<td>0.6</td>
<td>0.8</td>
<td>1.0</td>
</tr>
</tbody>
</table>
$^7\text{Li} \ (n,T) - \text{ENDF/B-VII: in } \Delta_{1g} \text{ for SL1}$

Cross-sections collapsed in 1 group with SL1

<table>
<thead>
<tr>
<th>XS MTs_1g</th>
<th>MT853</th>
<th>MT854</th>
<th>MT855</th>
<th>MT856</th>
<th>MT857</th>
<th>MT858</th>
<th>MT859</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.12E-03</td>
<td>4.76E-02</td>
<td>1.48E-02</td>
<td>2.10E-02</td>
<td>2.71E-02</td>
<td>1.53E-02</td>
<td>2.19E-33</td>
<td></td>
</tr>
</tbody>
</table>

MTs/MTtotal

0.05  0.36  0.11  0.16  0.20  0.12  0.00

Relative cocarivance matrix

<table>
<thead>
<tr>
<th>MT853</th>
<th>MT854</th>
<th>MT855</th>
<th>MT856</th>
<th>MT857</th>
<th>MT858</th>
<th>MT859</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.49E-03</td>
<td>0.00E+00</td>
<td>2.02E-04</td>
<td>-2.17E-06</td>
<td>-3.54E-05</td>
<td>-2.22E-05</td>
<td>-5.78E-20</td>
</tr>
<tr>
<td>0.00E+00</td>
<td>1.15E-03</td>
<td>-3.16E-04</td>
<td>-4.86E-04</td>
<td>-6.74E-04</td>
<td>-3.38E-04</td>
<td>-7.81E-18</td>
</tr>
<tr>
<td>2.02E-04</td>
<td>-3.16E-04</td>
<td>1.56E-03</td>
<td>1.70E-04</td>
<td>-1.42E-04</td>
<td>-7.21E-05</td>
<td>-5.10E-19</td>
</tr>
<tr>
<td>-2.17E-06</td>
<td>-4.86E-04</td>
<td>1.70E-04</td>
<td>2.07E-03</td>
<td>-2.60E-04</td>
<td>-1.25E-04</td>
<td>-1.36E-18</td>
</tr>
<tr>
<td>-3.54E-05</td>
<td>-6.74E-04</td>
<td>-1.42E-04</td>
<td>-2.60E-04</td>
<td>2.11E-03</td>
<td>2.24E-04</td>
<td>-2.97E-18</td>
</tr>
<tr>
<td>-2.22E-05</td>
<td>-3.38E-04</td>
<td>-7.21E-05</td>
<td>-1.25E-04</td>
<td>2.24E-04</td>
<td>3.16E-03</td>
<td>3.10E-17</td>
</tr>
<tr>
<td>-5.78E-20</td>
<td>-7.81E-18</td>
<td>-5.10E-19</td>
<td>-1.36E-18</td>
<td>-2.97E-18</td>
<td>3.10E-17</td>
<td>0.00E+00</td>
</tr>
</tbody>
</table>

Relative error(%) covariance matrix

<table>
<thead>
<tr>
<th>MT853</th>
<th>MT854</th>
<th>MT855</th>
<th>MT856</th>
<th>MT857</th>
<th>MT858</th>
<th>MT859</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.99</td>
<td>0.00</td>
<td>1.42</td>
<td>0.15</td>
<td>0.59</td>
<td>0.47</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>3.39</td>
<td>1.78</td>
<td>2.20</td>
<td>2.60</td>
<td>1.84</td>
<td>0.00</td>
</tr>
<tr>
<td>1.42</td>
<td>1.78</td>
<td>3.95</td>
<td>1.31</td>
<td>1.19</td>
<td>0.85</td>
<td>0.00</td>
</tr>
<tr>
<td>0.15</td>
<td>2.20</td>
<td>1.31</td>
<td>4.55</td>
<td>1.61</td>
<td>1.12</td>
<td>0.00</td>
</tr>
<tr>
<td>0.59</td>
<td>2.60</td>
<td>1.19</td>
<td>1.61</td>
<td>4.59</td>
<td>1.50</td>
<td>0.00</td>
</tr>
<tr>
<td>0.47</td>
<td>1.84</td>
<td>0.85</td>
<td>1.12</td>
<td>1.50</td>
<td>5.62</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

Rel. Err. in 1g (%) 1.17

The relative error in 1 group “lumped XS“ is only 1.17% !!!
$^6\text{Li}(n,T)$ - ENDF/B-VII vs EAF2010

Incident neutron data // Li6 //

- ENDF/B-VII
- EAF2007-PENDF
- EAF2010-VITJ175

Incident energy (MeV)

Grouped cross section (b)
$^6$Li(n,T) – EAF 2010/2007 and SCALE6.0: Covariance matrix

**EAF2010**

- Δσ/σ vs. E for $^6$Li(n,t)
  - Ordinate scales are % relative standard deviation and barns.
  - Abscissa scales are energy (eV).

**SCALE6.0**

- Δσ/σ vs. E for $^6$Li(n,t)
  - Ordinate scales are % relative standard deviation and barns.
  - Abscissa scales are energy (eV).
$^6\text{Li}(n,T)$ - ENDF/B-VII : Covariance Matrix in 44g

**ENDF/B-VII**

**Ordinate scales are % relative standard deviation and barns.**

**Abscissa scales are energy (eV).**

<table>
<thead>
<tr>
<th>Uncert_1group (ENDF/B-VII)</th>
<th>$\Delta^2_{\text{ENDF/B-VII}}$</th>
<th>Relative Exp Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^6\text{Li}(n,T)\text{He}_4$</td>
<td>6.64E-06</td>
<td>0.26</td>
</tr>
<tr>
<td>$^6\text{Li}(n,T)\text{He}_4$</td>
<td>1.59E-06</td>
<td>0.13</td>
</tr>
</tbody>
</table>
Objective:

“Processing and testing TENDL2010/EAF and TENDL2010/ENDF to activation calculations”

- Processing EAF/TENDL2010

  - Problems:
    - MT=18 and MT=102 with more than 10000 energy points
    - Different channels in the variance and cross section files
    - No uncertainties for isomeric/branching reactions

- Processing ENDF/TENDL2010

  - Problem:
    - NJOY/ERRORR-URR for Pu240
$^7\text{Li(}n,T\text{) – TENDL2010}$

EAF2010: Relative Error $\sim 33\%$

EAF2007-PENDF

TENDL2010/EAF

TENDL2010/ENDF

Incident neutron data \( / / \text{Li}^7 \) /
$^6\text{Li}(n,T) - \text{TENDL2010}$

Incident neutron data / $^6\text{Li}$ / MT=105 : (z,t) /

- TENDL2010/EAF
- TENDL2010/ENDF
- EAF2007-PENDF

Incident energy (MeV)

Cross-section (b)

JEFF/EFF Meeting May 2011

NEA, Paris, France
240Pu(n,γ) – EAF2007 vs TENDL2010/EAF

These are related to not-accurate-resonance widths
$^{240}$Pu(n,γ) – EAF2007 vs TENDL2010/EAF

Incident neutron data / Pu240 / MT=102 : (z,g) radiative capture / Cross section + Variance (R)

Incident energy (MeV) vs Cross-section (mb)
$^{240}\text{Pu}(n,\gamma)$ Covariance Matrix in 44g

EAF2010

SCALE6.0

Ordinate scales are % relative standard deviation and barns.
Abscissa scales are energy (eV).

Correlation Matrix

1.0  0.8  0.6  0.4  0.2  0.0  -0.2  -0.4  -0.6  -0.8  -1.0

Correlation Matrix

1.0  0.8  0.6  0.4  0.2  0.0  -0.2  -0.4  -0.6  -0.8  -1.0
$^{240}\text{Pu}(n,\gamma)$ Covariance Matrix in 44g

**TENDL2010/ENDF**

- Ordinate scales are % relative standard deviation and barns.
- Abscissa scales are energy (eV).

**TENDL2010/EAF**

- Ordinate scales are % relative standard deviation and barns.
- Abscissa scales are energy (eV).

ENDF files (where MF32 and MF33 are used)

EAF uncertainties come from Talys (Optical model): no resonance

info (no structure at low energy)
$^{240}\text{Pu}(n,\gamma)$ Covariance Matrix in 44g from RANDOM/EAF

How can we calculate the correlation matrix based on the random files?

TENDL2010/RANDOM EAF files
\(^{240}\text{Pu}(n,\gamma)\) Covariance Matrix in 44g

**TENDL2010/ENDF**

There is an overlap between the URR and the fast range (the URR goes from 5.7 keV to 40 keV and the fast range start at 5.7 keV).

**TENDL2010/RANDOM EAF files**

Can this effect explain part of the differences between TMC (using random files) and S/U methodologies (using ENDF covariances)?