Evaluation of ENDF/B-VIII Covariance Data

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Mini-CSEWG

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Overview

• Three general categories of testing performed
  – Two focus on uncertainty in $k_{\text{eff}}$ due to cross section covariance data
  – Other examines $c_k$ (similarity) of a reference set of experiments with reference applications

• Each test will be presented
  – Purpose: What is this test assessing and why is the test important?
  – Methodology: How is it done and what are the metrics?
  – Results: How do the results look for the ENDF/B-VIII covariance data?
    • Covariance library generated by Doro Wiarda based on data in repository on April 17
Caveats

• Technical
  – Sensitivity data used in testing was generated in SCALE 6.1 using ENDF/B-VII.0 cross sections
    • Covariance library contains relative uncertainties, so should be applicable regardless
    • Results support that testing is effective even with old sensitivity data because they are stationary with respect to the data changes – change one thing at a time!
    • Plan to regenerate sensitivity data with SCALE 6.2.2 & ENDF/B-VII.1 this year

• Less technical
  – I am not a nuclear data expert; I’m a criticality safety applications guy
  – As will become clear, I believe the covariances are too large
  – Do not take anything I say as a personal attack on your work
Cross section uncertainty for critical experiments

• Purpose:
  – Generate $k_{\text{eff}}$ uncertainty due to covariances for critical experiments in VALID library maintained at ORNL
  – Compare variability of predictions with resulting uncertainty band
  – Plots frequently presented by Mark Williams, Brad Rearden, and others

• Methodology:
  – TSUNAMI-IP will calculate $k_{\text{eff}}$ uncertainty resulting from covariance data
    • Covariance patching turned off for data testing
    • “uncert” and “values” keywords in parameters block
  – Covariances propagated with sensitivities to determine uncertainty in $k_{\text{eff}}$
  – Detailed uncertainty edit can also be generated for each element in the covariance matrix
Results: HEU-MET-FAST

- 49 critical configurations
- C/E plotted for 252-group ENDF/B-VII.1 library
- Error bar is $1\sigma$ experimental uncertainty
- X variable is case number: no attempt to find trends
- HMF cases have generally not shown much impact in either ENDF/B-VII.1 or ENDF/B-VIII
Results: LEU-COMP-THERM

- 140 critical configurations
- C/E and error bar same as previous plot
- Noticeably larger uncertainty band with ENDF/B-VIII than SCALE 6.2.1
- Traced to $^{235}\text{U}$ nubar and $^{1}\text{H}$ capture and scatter
  - Reintroduction of errors identified in ENDF/B-VII.1 data during preparation and testing of SCALE 6.2 covariance library
Results: MIX-COMP-THERM

- 49 critical configurations
- New zigzag in the middle of the data is caused by $^1$H capture
- Generally fewer points outside the uncertainty band for Pu-fueled systems in SCALE 6.2 and beyond
  - MCT-008 appears biased low, especially Cases 7-28
- Uncertainty may be creeping back – or is it just the $^1$H problem?
Results: PU-SOL-THERM

- 81 critical configurations
- $^{239}\text{Pu}$ covariance data missing, so not tested
  - Obviously would have large impact here
- Again, results looked better with $^{239}\text{Pu}$ nubar from ENDF/B-VII.1
  - Is that unrealistically low?
## Results: Summary Table

<table>
<thead>
<tr>
<th>Category</th>
<th>Number of Cases</th>
<th>Avg C/E (CE_V7.1)</th>
<th>Avg Exp. Unc.</th>
<th>St. Dev. Of C/Es</th>
<th>Avg 1σ XS Unc</th>
<th>% of Cases Within</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
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<td>SCALE 6.2</td>
<td>E8+SCALE</td>
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<tr>
<td>HMF</td>
<td>49</td>
<td>1.00014</td>
<td>194</td>
<td>477</td>
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<td>1474</td>
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<td>1288</td>
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<td>1591</td>
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<td>420</td>
<td>850</td>
<td>995</td>
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</tbody>
</table>

The cross section uncertainty band is **TOO WIDE**!
The experimental uncertainty band is in generally good agreement with the observed variability.
Questions before we move on?
Cross section uncertainty for SNF

• Purpose:
  – Determine $k_{\text{eff}}$ uncertainty for each isotope in an SNF storage/transportation configuration, then also combine into specific groups
  – Major/minor/other actinides, major/other fission products, else/structural
  – Supported NRC Interim Staff Guidance 8, Revision 3 (ISG-8R3): PWR BUC

• Methodology:
  – TSUNAMI-IP will calculate $k_{\text{eff}}$ uncertainty resulting from covariance data for each element in the covariance matrix (isotope/reaction pair and cross terms)
    • “uncert_long” keyword in parameters block
  – AWK script combines uncertainty components for each isotope
  – Spreadsheet used to collect information by category
# Results

<table>
<thead>
<tr>
<th>Category</th>
<th>PWR Spent Fuel Pool Model</th>
<th>PWR Spent Fuel Cask Model</th>
<th>BWR SFP Model</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>10 GWd/MTU</td>
<td>40 GWd/MTU</td>
<td>10 GWd/MTU</td>
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<td></td>
<td>6.2 E8+</td>
<td>6.2 E8+</td>
<td>6.2 E8+</td>
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<td>Maj. Act.</td>
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<td>ALL % Diff</td>
<td>(E8-6.2)/6.2</td>
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</tbody>
</table>
Results: Isotopes that caused differences

- Major actinides: $^{235}\text{U}$ and $^{240}\text{Pu}$
- Major fission products: $^{149}\text{Sm}$ and $^{151}\text{Sm}$; $^{103}\text{Rh}$ to a lesser extent
- Other actinides: $^{233}\text{U}$ (11,000% to 25,000% increase)
- Other fission products: $^{147}\text{Pm}$ (Almost a factor of 4)
- Else/structural: $^1\text{H}$
Questions before we move on?
\( c_k \) (similarity) assessment

**Purpose:**
- Calculate \( c_k \) parameter for each experiment in a reference set compared to multiple spent fuel storage/transportation applications
- What is \( c_k \)?
  - Correlation coefficient between an experiment and an application based on shared nuclear data uncertainty

\[
C_{aa} = \frac{\text{COV}(\alpha_m, \alpha_p)}{\alpha_m \alpha_p}, \quad m = 1, 2, ..., M, \quad p = 1, 2, ..., M
\]

Covariance data

\[
S_k = \frac{\alpha_m, \frac{\partial \alpha_i}{\partial \alpha_m}}{k_i}, \quad i = 1, 2, ..., I, \quad m = 1, 2, ..., M
\]

Sensitivity data

Uncertainty matrix:

\[
C_{kk} = S_k C_{aa} S_k^T
\]

Given:

\[
c_k = \frac{\sigma_{ij}^2}{(\sigma_i \sigma_j)^2}
\]

Where:
- \( \sigma_{ij}^2 \) is off-diagonal term of \( C_{kk} \) matrix (aka covariance)
- \( \sigma_i \) and \( \sigma_j \) are square root of diagonal terms (aka standard deviations)
\( c_k \) (similarity) assessment (2)

- **Purpose (continued):**
  - How is it useful in covariance testing?
    - \( c_k \) can indicate which covariance data are important in determining similarity
    - Results should be explicable result of composition of systems
    - Especially helpful for comparison of primary fissile species uncertainty data

- **Methodology:**
  - TSUNAMI-IP calculates \( c_k \) provided sensitivity data files (SDFs) for each application and experiment
  - “c” and “values” keywords in parameter block
  - “c_long” is also helpful because it provides the \( c_k \) contribution from each element in the covariance matrix
$c_k$ results – historical context: SCALE 6.1 to SCALE 6.2

- 1643 unique critical experiments
- PWR SNF cask with fuel at representative discharge burnup
- SCALE 6.1 (purple)
- SCALE 6.2 (various)
- This change caused significant turmoil for use of $c_k$ to select similar experiments for validation.
• Same critical experiments and PWR SNF
• SCALE 6.2 (various)
• ENDF/B-VIII plus SCALE data (black)

This change further reduces MCT systems and increases LCT systems. The result doesn’t make sense – LEU can’t be representative of SNF.
**c_k summary**

- Increased $^{235}\text{U}$ nubar uncertainty results in higher similarity for LCT systems with SNF storage/transportation models
  - This exacerbates a change resulting from ENDF/B-VII.1 covariance changes to $^{235}\text{U}$ (bigger) and $^{239}\text{Pu}$ (smaller)

- Without reliable covariance data, S/U methods cannot be used to select appropriate experiments for validation
  - Reliability of covariance data is also a significant problem for data adjustment methods (e.g., TSURFER)
Overall testing summary & conclusions

- $^{235}$U nubar and $^1$H covariance data has regressed to incorrect values included in ENDF/B-VII.1 and previously identified by ORNL

- There was no $^{239}$Pu covariance data in ENDF/B-VIII when Doro pulled the data, so the SCALE 6.2 value was used
  - No indication of how ENDF/B-VIII $^{239}$Pu covariance data perform

- Uncertainty bands have historically been too wide, and still tend to increase and not decrease with each new release

- Inappropriate uncertainty bands undermine usefulness of S/U methods for criticality safety validation, reactor physics uncertainty quantification, and depletion calculation uncertainty quantification
This concludes my prepared remarks. Are there any additional questions at this time?

marshallwj@ornl.gov if you have additional questions at a later date.

Thank you for your attention!
h-1 mt=102 n,\gamma - Std dev by energy

- h-1 mt=102 n,\gamma ENDF/B-VIII
- h-1 mt=102 n,\gamma SCALE 6.2.1
Results: Summary Table $\chi^2$

<table>
<thead>
<tr>
<th>Category</th>
<th>Number of Cases</th>
<th>$\chi^2$ Statistic (Should $\approx$ Num. of Cases)</th>
<th>$\chi^2$ P-Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>HMF</td>
<td>49</td>
<td>7.94</td>
<td>1.000000000000</td>
</tr>
<tr>
<td>HST</td>
<td>52</td>
<td>10.93</td>
<td>0.99999999996</td>
</tr>
<tr>
<td>IMF</td>
<td>13</td>
<td>2.62</td>
<td>0.9976738347</td>
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<tr>
<td>LCT</td>
<td>140</td>
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<td>LST</td>
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<td>PMF</td>
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