Sensitivity/uncertainty Analysis Applied to the Phase VII Benchmark

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\(^{(3)}\) SEA Ingeniería Análisis de Blindaje, S.L.

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CONCLUSIONS
Phase-VII Benchmark

“The main objective of this benchmark is to study the ability of relevant computer codes and associated nuclear data to predict spent fuel isotopic compositions and corresponding $k_{\text{eff}}$ values in a cask configuration over the time duration relevant to spent nuclear fuel disposal, out to 1 000 000 years”

Our main contribution involves:

- ACAB code for inventory prediction (NEA-1839: ACAB-2008, ACtivation ABacus Code)
- MCNP5 for criticality calculation
- JEFF-3.1.1 nuclear data library (decay and neutron transport libraries)

Sensitivity study

- Isotopic inventory: Decay data libraries (ORIGEN-S, ORIGEN2.2), impact of numerical solvers and time-step
- Criticality calculations: different isotopic inventories, neutron transport codes (KENO-VI) and neutron transport libraries (ENDF/B-VI)

Sensitivity/uncertainty assessment

- Sensitivity profiles of concentration and multigroup cross-section for the main fuel isotopes
- Global uncertainty assessment: decay data and activation cross section data
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CONCLUSIONS
The Benchmark specifications provide the discharge fuel composition (4.5 initial wt% $^{235}$U, 50GWD/MTU) for calculating time-dependent spent fuel compositions.


1) **Decay calculation:**

The discharge fuel composition provided contains 113 nuclides: Benchmark nuclides (53) and their precursors (60) that are relevant to the decay calculations.

Those 53 **Benchmark nuclides** (light element, actinide, and fission product) were selected according to its relevance to burnup-credit criticality calculations and those that are potential contributors to radiation dose to the public from nuclear waste repositories.

2) **Criticality calculation:**

Providing $k_{\text{eff}}$ values for fresh fuel and isotopic compositions from the decay calculations (30 post-irradiation time steps, out to 1 000 000 years) for two cases involving a first set (**ACT**) of 11 actinides and a second case (**PFs**) involving 14 actinides and 16 fission products.

The criticality model for $k_{\text{eff}}$ calculations is a representative cask loaded with 21 PWR-UO2 17×17 fuel assemblies.
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2.1. Benchmark results: Decay calculations

FIG 1. Evolution of the main actinides selected in the actinide-only burnup-credit nuclide set. Calculation performed with ACAB code and JEFF-3.1.1 decay data library.

- **Pu\textsuperscript{241} (T\textsubscript{1/2}=14.3 y)**, **Pu\textsuperscript{240} (T\textsubscript{1/2}=6.56E+3 y)** and **Pu\textsuperscript{239} (T\textsubscript{1/2}=2.41E+4 y)**
- **Am\textsuperscript{241} (T\textsubscript{1/2}=433 y)**: \( Pu\textsuperscript{241}(\beta-)Am\textsuperscript{241} \)
- **U\textsuperscript{235}**: increases the concentration in a factor of 1.76, the main reaction is \( Pu\textsuperscript{239}(\alpha)U\textsuperscript{235} \)
- **U\textsuperscript{233}**: \( Pu\textsuperscript{241}(\beta-)Am\textsuperscript{241}(\alpha)Np\textsuperscript{237}(\alpha)Pa\textsuperscript{233}(\beta-)U\textsuperscript{233} \) & \( Np\textsuperscript{237}(\alpha)Pa\textsuperscript{233}(\beta-)U\textsuperscript{233} \)
For decay calculations, we have performed a decay sensitivity analysis assessing the importance of decay nuclear data and numerical solvers implemented in ACAB code.

### 1) Impact of different nuclear decay data libraries
- Significant differences: JEFF-3.1.1 vs ORIGEN2.2
- Good agreement: JEFF-3.1.1 vs ORIGEN_S

### 2) Importance of numerical solvers
- ACAB with LSODE solver: Only differences in Pb$^{210}$ (~6%) and Ra$^{228}$ (~3%) were found
- Analysis of a reduced time-step calculation (ACAB pulsed option) has shown discrepancies (< 10%) in Sb$^{126}$, Pb$^{210}$, Ac$^{227}$, Th$^{229}$, Pa$^{231}$ and U$^{233}$

#### Table I. Major differences between JEFF-3.1.1 and ORIGEN-S decay data contributing to the differences in the isotopic prediction for this Benchmark.

<table>
<thead>
<tr>
<th></th>
<th>JEFF-3.1.1</th>
<th>ORIGEN-S</th>
<th>Diff (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{1/2}$ Ni$^{59}$ (s)</td>
<td>2.3980E+12</td>
<td>2.3670E+12</td>
<td>-1.29</td>
</tr>
<tr>
<td>$T_{1/2}$ Se$^{79}$ (s)</td>
<td>1.1900E+13</td>
<td>9.3000E+12</td>
<td>-21.85</td>
</tr>
<tr>
<td>$T_{1/2}$ Sr$^{90}$ (s)</td>
<td>9.0850E+08</td>
<td>8.8830E+08</td>
<td>-2.22</td>
</tr>
<tr>
<td>Yield (Zr$^{93}$ to Nb$^{93m}$)</td>
<td>9.7500E-01</td>
<td>1.0000E+00</td>
<td>2.50</td>
</tr>
<tr>
<td>$T_{1/2}$ Nb$^{94}$ (s)</td>
<td>6.3070E+11</td>
<td>6.4060E+11</td>
<td>1.57</td>
</tr>
<tr>
<td>$T_{1/2}$ Mo$^{93}$ (s)</td>
<td>1.2620E+11</td>
<td>1.1045E+11</td>
<td>-12.55</td>
</tr>
<tr>
<td>$T_{1/2}$ Tc$^{99}$ (s)</td>
<td>6.7530E+12</td>
<td>6.6620E+12</td>
<td>-1.35</td>
</tr>
<tr>
<td>$T_{1/2}$ Sn$^{126}$ (s)</td>
<td>7.2580E+12</td>
<td>3.1558E+12</td>
<td>-56.52</td>
</tr>
<tr>
<td>$T_{1/2}$ I$^{129}$ (s)</td>
<td>5.0810E+14</td>
<td>4.9540E+14</td>
<td>-2.49</td>
</tr>
<tr>
<td>$T_{1/2}$ Eu$^{155}$ (s)</td>
<td>1.5000E+08</td>
<td>1.4770E+08</td>
<td>-1.53</td>
</tr>
<tr>
<td>$T_{1/2}$ Th$^{229}$ (s)</td>
<td>2.3160E+11</td>
<td>2.4870E+11</td>
<td>7.38</td>
</tr>
<tr>
<td>$T_{1/2}$ U$^{236}$ (s)</td>
<td>7.4790E+14</td>
<td>7.3910E+14</td>
<td>-1.17</td>
</tr>
<tr>
<td>$T_{1/2}$ Pu$^{236}$</td>
<td>9.0190E+07</td>
<td>9.1520E+07</td>
<td>1.47</td>
</tr>
</tbody>
</table>
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CONCLUSIONS
For **criticality calculations**, a representative PWR cask model is selected to predict $k_{\text{eff}}$

- Computing tools: MCNP5 and KENO-VI
- Nuclear Data libraries: JEFF-3.1.1, ENDF/B-VI

**Table II.** Different cases for inventory prediction and criticality calculations.

<table>
<thead>
<tr>
<th>Cases #</th>
<th>Isotopic prediction: ACAB code using different decay library</th>
<th>$k_{\text{eff}}$ prediction: different neutron transport libraries and codes</th>
<th>$k_{\text{eff}}$ (fresh fuel)</th>
<th>$k_{\text{eff}}$ (shutdown)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (reference)</td>
<td>JEFF-3.1.1</td>
<td>MCNPX-JEFF-3.1.1</td>
<td>1.15057 ± 0.00035</td>
<td>0.95819 ± 0.00033</td>
</tr>
<tr>
<td>2</td>
<td>JEFF-3.1.1</td>
<td>MCNPX-ENDF/B-VI</td>
<td>1.14631 ± 0.00053</td>
<td>0.95228 ± 0.00050</td>
</tr>
<tr>
<td>3</td>
<td>JEFF-3.1.1</td>
<td>SCALE6-ENDF/B-V-44groups</td>
<td>1.14688 ± 0.00009</td>
<td>0.95737 ± 0.00008</td>
</tr>
<tr>
<td>4</td>
<td>ORIGEN-2.2</td>
<td>MCNPX-ENDF/B-VI</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>5</td>
<td>ORIGEN-S</td>
<td>MCNPX-JEFF-3.1.1</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
FIG 2. The calculated $k_{\text{eff}}$ values for actinide case (ACT).

(I = Decay data library for the isotopic inventory; NT= Neutron transport library for $k_{\text{eff}}$ calculation)

- $k_{\text{eff}}$ has a maximum value at shutdown
- Minimum value at 100 years
- $k_{\text{eff}}$ increases to another maximum around 30,000 years cooling time, this second maximum is always below the $k_{\text{eff}}$ at shutdown
The isotopic calculations performed with ACAB code with different decay data libraries: $k_{\text{eff}}$ prediction < 200 pcm

Significant differences between JEFF-3.1.1 and ENDF/B-VI: 400-760 pcm: due to $^{238}\text{U}$ and $^{241}\text{Am}$
Table III. \( \Delta k_{\text{eff}} \) (ENDF/B-VI-JEFF-3.1.1) predicted by substituting individual isotopes with those of the ENDF/B-VI in the reference \( k_{\text{eff}} \) calculation performed with JEFF-3.1.1.

<table>
<thead>
<tr>
<th></th>
<th>Shutdown</th>
<th>100 years</th>
<th>1E+06 years</th>
</tr>
</thead>
<tbody>
<tr>
<td>U233</td>
<td>-0.00034</td>
<td>-0.00020</td>
<td>-0.00034</td>
</tr>
<tr>
<td>U234</td>
<td>-0.00040</td>
<td>-0.00002</td>
<td>0.00009</td>
</tr>
<tr>
<td>U235</td>
<td>0.00060</td>
<td>0.00137</td>
<td>0.00219</td>
</tr>
<tr>
<td>U236</td>
<td>-0.00111</td>
<td>-0.00033</td>
<td>0.00043</td>
</tr>
<tr>
<td>U238</td>
<td>-0.00581</td>
<td>-0.00478</td>
<td>-0.00611</td>
</tr>
<tr>
<td>Pu238</td>
<td>0.00030</td>
<td>-0.00001</td>
<td>0.00000</td>
</tr>
<tr>
<td>Pu239</td>
<td>0.00072</td>
<td>0.00208</td>
<td>0.00079</td>
</tr>
<tr>
<td>Pu240</td>
<td>-0.00198</td>
<td>-0.00071</td>
<td>0.00051</td>
</tr>
<tr>
<td>Pu241</td>
<td>0.00199</td>
<td>0.00113</td>
<td>-0.00030</td>
</tr>
<tr>
<td>Pu242</td>
<td>-0.00121</td>
<td>-0.00017</td>
<td>0.00011</td>
</tr>
<tr>
<td>Am241</td>
<td>-0.00032</td>
<td>0.00552</td>
<td>-0.00030</td>
</tr>
</tbody>
</table>

This discrepancy can be explained by the differences in the resolved resonance parameters between ENDF/B-VI and JEFF-3.1.1 resulting:

- lower \( U^{238} \) resonance absorption
- higher neutron spectrum in the resonance energy region

2.2 Benchmark Results: Criticality calculations

![Graph showing differences in flux and XS]
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CONCLUSIONS
Goal: to analyse how DECAY DATA (\(\lambda\)s, BRs) uncertainty is transmitted to X

\[
\frac{d}{dt} X = AX
\]

\[
X = (X_1, X_2, \ldots)
\]

\[
X_i = X_i(\lambda, \text{branching ratio})
\]

1) Sensitivity / Uncertainty Analysis (S/U)

Method based on the first order Taylor series to estimate uncertainty indices for each \(\lambda\) and branching ratio in a cooling scenario

2) Monte Carlo Uncertainty Analysis (MC)

To treat the global effect of all decay data uncertainties in activation calculations, we have proposed an uncertainty analysis methodology based on Monte Carlo random sampling of the decay data (\(\lambda\) and branching ratios)

Assignment of a Probability Density Function (PDF) to each decay data

3) Propagation of uncertainties in decay calculations based on S/U and MC approaches
Sensitivity Analysis

\[ X_i(\lambda) \approx X_i(\lambda_0) + \sum_{j=1}^{m} \left[ \frac{\partial X_i}{\partial \lambda_j} \right]_{\sigma_0} (\lambda_j - \lambda_{j0}) \]

\[ \frac{X_i(\lambda) - X_i(\lambda_0)}{X_i(\lambda_0)} \approx \sum_{j=1}^{m} \frac{\lambda_{j0}}{X_i(\lambda_0)} \left[ \frac{\partial X_i}{\partial \lambda_j} \right]_{\sigma_0} (\lambda_j - \lambda_{j0}) \]

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

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

\[ \text{Var}[e_i] = \rho_i^T M \rho_i \]

\[ \rho_i = \begin{pmatrix} \rho_{i1} & \rho_{i2} & \cdots & \rho_{im} \end{pmatrix} \]

\[ \varepsilon_j \]

Relative error in \( X_i \) due to changes in decay data \( \lambda \)

Sensitivity coefficient

Relative error in decay data \( \lambda_j \)

Information obtained processing JEFF-3.1.1
Monte Carlo method

- We use simultaneous random sampling of all the Decay Data PDFs involved in the problem
- PDF is assigned to each $\lambda_j$: $\varepsilon_j \rightarrow N(0, \Delta_j)$

$$\
\begin{pmatrix}
    \lambda_1 - \lambda_{i10} \\
    \lambda_{i10} \\
    \lambda_2 - \lambda_{i20} \\
    \lambda_{i20} \\
    \vdots \\
    \lambda_m - \lambda_{im0} \\
    \lambda_{im0}
\end{pmatrix} \rightarrow N(0, M)
$$

- From the sample of the random vector $\lambda$, $\lambda = (\lambda_1, ..., \lambda_j, ..., \lambda_m)$ the matrix $A$ is computed and the vector of nuclide quantities $X$ is obtained $X = (X_1, ..., X_i, ..., X_n)$

- 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 $\Delta \lambda$ on $X$
## Table IV. Half-life and relative errors (in %) from JEFF-3.1.1 decay data library

<table>
<thead>
<tr>
<th>Isotope</th>
<th>$T_{1/2}$ (y)</th>
<th>Err(%)</th>
<th>Isotope</th>
<th>$T_{1/2}$ (y)</th>
<th>Err(%)</th>
<th>Isotope</th>
<th>$T_{1/2}$ (y)</th>
<th>Err(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C 14</td>
<td>5.7007E+03</td>
<td>0.53</td>
<td>CS135</td>
<td>2.2999E+06</td>
<td>13.04</td>
<td>U233</td>
<td>1.5926E+05</td>
<td>0.13</td>
</tr>
<tr>
<td>CL 36</td>
<td>3.0101E+05</td>
<td>1.00</td>
<td>CS137</td>
<td>3.0040E+01</td>
<td>0.10</td>
<td>U234</td>
<td>2.4571E+05</td>
<td>0.12</td>
</tr>
<tr>
<td>CA 41</td>
<td>1.0299E+05</td>
<td>3.88</td>
<td>SM147</td>
<td>1.0600E+11</td>
<td>1.89</td>
<td>U235</td>
<td>7.0379E+08</td>
<td>0.07</td>
</tr>
<tr>
<td>NI 59</td>
<td>7.5988E+04</td>
<td>6.58</td>
<td>SM149</td>
<td>2.0002E+15</td>
<td>0.00</td>
<td>U236</td>
<td>2.3700E+07</td>
<td>0.84</td>
</tr>
<tr>
<td>SE 79</td>
<td>3.7709E+05</td>
<td>5.04</td>
<td>SM151</td>
<td>8.9994E+01</td>
<td>6.67</td>
<td>U238</td>
<td>4.4680E+09</td>
<td>0.07</td>
</tr>
<tr>
<td>SR 90</td>
<td>2.8789E+01</td>
<td>0.21</td>
<td>PB210</td>
<td>2.2159E+01</td>
<td>0.54</td>
<td>NP237</td>
<td>2.1399E+06</td>
<td>0.47</td>
</tr>
<tr>
<td>ZR 93</td>
<td>1.5299E+06</td>
<td>6.54</td>
<td>RA226</td>
<td>1.5999E+03</td>
<td>0.44</td>
<td>PU238</td>
<td>8.7713E+01</td>
<td>0.34</td>
</tr>
<tr>
<td>NB 93M</td>
<td>1.6126E+01</td>
<td>0.85</td>
<td>RA228</td>
<td>5.7514E+00</td>
<td>0.52</td>
<td>PU239</td>
<td>2.4111E+04</td>
<td>0.05</td>
</tr>
<tr>
<td>NB 94</td>
<td>1.9986E+04</td>
<td>12.33</td>
<td>AC227</td>
<td>2.1773E+01</td>
<td>0.01</td>
<td>PU240</td>
<td>6.5626E+03</td>
<td>0.08</td>
</tr>
<tr>
<td>MO 93</td>
<td>3.9990E+03</td>
<td>20.00</td>
<td>TH229</td>
<td>7.3390E+03</td>
<td>2.18</td>
<td>PU241</td>
<td>1.4329E+01</td>
<td>0.28</td>
</tr>
<tr>
<td>TC 99</td>
<td>2.1399E+05</td>
<td>3.74</td>
<td>TH230</td>
<td>7.5386E+04</td>
<td>0.40</td>
<td>PU242</td>
<td>3.7360E+05</td>
<td>0.29</td>
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<tr>
<td>PD107</td>
<td>6.4992E+06</td>
<td>4.61</td>
<td>TH232</td>
<td>1.4050E+10</td>
<td>0.43</td>
<td>AM241</td>
<td>4.3286E+02</td>
<td>0.16</td>
</tr>
<tr>
<td>SN126</td>
<td>2.2999E+05</td>
<td>6.09</td>
<td>PA231</td>
<td>3.2765E+04</td>
<td>0.34</td>
<td>AM242M</td>
<td>1.4101E+02</td>
<td>1.42</td>
</tr>
<tr>
<td>SB126</td>
<td>3.3938E-02</td>
<td>0.81</td>
<td>U232</td>
<td>6.9809E+01</td>
<td>0.72</td>
<td>AM243</td>
<td>7.3643E+03</td>
<td>0.30</td>
</tr>
<tr>
<td>SB126M</td>
<td>3.6315E-05</td>
<td>1.05</td>
<td></td>
<td></td>
<td></td>
<td>CM245</td>
<td>8.4987E+03</td>
<td>2.35</td>
</tr>
<tr>
<td>I129</td>
<td>1.6101E+07</td>
<td>4.35</td>
<td></td>
<td></td>
<td></td>
<td>CM246</td>
<td>4.7310E+03</td>
<td>3.17</td>
</tr>
</tbody>
</table>
The overall uncertainty analysis by a general Monte Carlo procedure:

FIG 4. Concentrations and rel. error (in %) in the isotopic prediction of $^{233,234,235,236}$U and $^{238}$U.

Only a few set of isotopes have shown errors larger than 1% to be taken into account:

i) activation/fiss. products: $^{41}$Ca, $^{59}$Ni, $^{79}$Se, $^{93m}$Nb, $^{94}$Nb, $^{93}$Mo, $^{99}$Tc, $^{126}$Sn, $^{126}$Sb, $^{126m}$Sb, $^{151}$Sm, $^{151}$Eu

ii) actinides: $^{242m}$Am, $^{245}$Cm, $^{246}$Cm
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CONCLUSIONS
Forward Error Propagation to:

“Determine the accuracy of $k_{\text{eff}}$ calculation due to the uncertainties in the basic data”
- Decay data
- Cross section data

1) **$k_{\text{eff}}$ sensitivity profiles**

Change in $k_{\text{eff}}$ due to a relative change in:

i) Atomic density for the relevant isotope-i: $\Delta k/(\Delta N_i/N_i)$
ii) Cross-section in energy group-g: $\Delta k/(\Delta \sigma_g/\sigma_g)$

These sensitivity profiles are obtained using the perturbation option of MCNP (invoked with the PERT-card with the default option (i.e. method = 1))

2) The sensitivity profile ($S_{k_{\text{eff}}}$) thus produced by MCNP and the relevant variance/covariance matrices ($D$) can be used to carry out an **uncertainty calculation**.

$$\Delta k_{\text{eff}}^2 = S_{k_{\text{eff}}}^+ \cdot D \cdot S_{k_{\text{eff}}}$$

3) **Variance/covariance matrices ($D$)**

i) Relative error in $\Delta N$ predicted due to the uncertainty in decay data (see **PART II**)
ii) Relative error in cross-section data (e.g. BOLNA)
FIG. 5. The $k_{eff}$ evolution and $k_{eff}$ sensitivity profiles due to a relative change of 1% in the atomic density for the main fuel isotopes at shutdown.

Calculations performed for the case of actinide-only (ACT) burnup-credit nuclides.
FIG. 6. $k_{\text{eff}}$ evolution and $k_{\text{eff}}$ sensitivity profiles for the two calculations performed in the Benchmark: actinide-only (ACT) and actinide+fission products (PFs) burnup-credit nuclides.

The uncertainty estimates in $k_{\text{eff}}$ due to decay data uncertainties is $< 10$ pcm
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FIG. 7. Sensitivity coefficient of the keff for $\sigma_c^{U238}$ at different cooling times ranging from shutdown up to 1.0E+6 years. Calculations performed for the case of actinide-only burnup-credit nuclides.

3.2.2 Error Propagation to “Criticality Calculations”: $\Delta X S_g$
FIG. 8. Sensitivity coefficients of the keff for $\sigma_{\text{fiss}}^{\text{Pu241}}$ at different cooling times ranging from shutdown up to $1.0\times10^6$ years. Calculations performed for the case of actinide-only burnup-credit nuclides.
BOLNA (15-energy-group structure): These uncertainties (diagonal values) are based as much as possible on the nuclear data performance in the analysis of selected, clean integral experiments (irradiated fuel and sample analysis, criticality and fission rates in zero-power critical facilities).


Table V. BOLNA variance matrix Pu\textsuperscript{239,241} and U\textsuperscript{238}
FIG. 9. Errors in $\Delta k_{eff}$ using BOLNA diagonal uncertainty by isotope and reaction. Calculations performed for the case of actinide-only (ACT) burnup-credit nuclides.

Two major data sources for the overall uncertainties (> 100 pcm) are identified:

1) Fission of $^{239}\text{Pu}$ and $^{241}\text{Pu}$
2) Capture for $^{238}\text{U}$, $^{239}\text{Pu}$, $^{240}\text{Pu}$ and $^{235}\text{U}$
FIG. 10. Errors in $k_{\text{eff}}$ using BOLNA diagonal uncertainty by isotope. Calculations performed for the case of actinide-only burnup-credit nuclides.

**Main conclusions:**

1) Relatively small uncertainties on $k_{\text{eff}}$ are observed (< 300 pcm):
   - Very small uncertainties are assumed on the low-energy data of:
     - $^{235}\text{U}$
     - $^{238}\text{U}$
     - $^{239}\text{Pu}$
     - $^{240}\text{Pu}$ capture close to the first resonance

2) Significant contributions, e.g. the $^{241}\text{Pu}$ fission
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The target accuracies in $\Delta k_{\text{eff}}$ can be achieved by reducing the uncertainties in some multigroup cross sections data ($\Delta \sigma_i$).

To evaluate the required reduction and establish priorities on data uncertainty reduction, an optimization problem is solved:

1) Minimization of the **objective function**: 

$$
\sum_{i=1}^{I} \frac{\lambda_i}{(\Delta \sigma_i)^2}
$$

where $I$ is the total number of parameters ($\sigma_{c_{U235}}$, $\sigma_{\text{fiss }U235}$, ...), $\lambda_i$ is the cost parameter, and $\Delta \sigma_i$ is the uncertainty.

2) **Unknown uncertainty data** requirements: $\Delta \sigma_i$

- Cost parameter: $\lambda_i = 1.0$

3) With the **constraints**:

$$
\Delta \sigma_i \geq 0
$$

$$
\Delta k_{\text{eff}} = \sqrt{\sum_{i=1}^{I} (\rho_i \Delta \sigma_i)^2} \leq (\delta_n)_{pcm}
$$

where $\delta_n$ is the design parameter uncertainties, $\rho_i$ are the correlation coefficients, and $n=1, \ldots, N$ (shutdown + cooling times) are the design parameters.

**NOTE**: Only diagonal values of the BOLNA covariance matrix have been used
### Table VI. Uncertainty reduction requirements needed to meet $\Delta k_{\text{eff}}$ parameter target accuracies.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Cross-section</th>
<th>Energy-range</th>
<th>Current Accuracy in BOLNA (%) (diagonal values)</th>
<th>Required $\Delta k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>U235</td>
<td>CAPT</td>
<td>0.54-0.10 eV</td>
<td>1.55</td>
<td>1.43 1.55 1.55 1.55</td>
</tr>
<tr>
<td></td>
<td></td>
<td>below 0.10 eV</td>
<td>1.73</td>
<td>0.58 1.29 1.73</td>
</tr>
<tr>
<td></td>
<td></td>
<td>24.8-9.12 keV</td>
<td><strong>9.43</strong></td>
<td>2.21 2.97 4.13</td>
</tr>
<tr>
<td></td>
<td></td>
<td>9.12-2.03 keV</td>
<td>3.11</td>
<td>1.28 2.14 2.94</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.03-0.454 keV</td>
<td>2.10</td>
<td>1.10 1.91 2.10</td>
</tr>
<tr>
<td>U238</td>
<td>CAPT</td>
<td>454.0-22.6 eV</td>
<td>1.71</td>
<td>0.69 1.16 1.60</td>
</tr>
<tr>
<td></td>
<td></td>
<td>22.6-4.0 eV</td>
<td>1.03</td>
<td>0.71 1.03 1.03</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.0-0.54 eV</td>
<td>2.45</td>
<td>1.69 2.45 2.45</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.54-0.10 eV</td>
<td>1.66</td>
<td>0.97 1.66 1.66</td>
</tr>
<tr>
<td></td>
<td></td>
<td>below 0.10 eV</td>
<td>1.64</td>
<td>0.44 0.82 1.14</td>
</tr>
<tr>
<td>PU239</td>
<td>FISS</td>
<td>0.54-0.10 eV</td>
<td>0.88</td>
<td>0.41 0.63 0.88</td>
</tr>
<tr>
<td></td>
<td></td>
<td>below 0.10 eV</td>
<td>1.11</td>
<td>0.34 0.52 0.74</td>
</tr>
<tr>
<td></td>
<td>CAPT</td>
<td>0.54-0.10 eV</td>
<td>1.36</td>
<td>0.54 0.83 1.14</td>
</tr>
<tr>
<td></td>
<td></td>
<td>below 0.10 eV</td>
<td>1.60</td>
<td>0.55 0.84 1.17</td>
</tr>
<tr>
<td>PU240</td>
<td>CAPT</td>
<td>0.54-0.10 eV</td>
<td>3.23</td>
<td>1.80 2.42 3.23</td>
</tr>
<tr>
<td></td>
<td></td>
<td>below 0.10 eV</td>
<td><strong>4.79</strong></td>
<td>0.89 1.36 1.89</td>
</tr>
<tr>
<td>PU241</td>
<td>FISS</td>
<td>454.0-22.6 eV</td>
<td><strong>19.38</strong></td>
<td>3.33 3.73 4.91</td>
</tr>
<tr>
<td></td>
<td></td>
<td>22.6-4.0 eV</td>
<td>4.21</td>
<td>2.12 2.63 3.47</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.54-0.10 eV</td>
<td>2.94</td>
<td>1.00 1.48 1.95</td>
</tr>
<tr>
<td></td>
<td></td>
<td>below 0.10 eV</td>
<td><strong>3.27</strong></td>
<td>0.67 0.97 1.28</td>
</tr>
<tr>
<td></td>
<td>CAPT</td>
<td>0.54-0.10 eV</td>
<td><strong>6.84</strong></td>
<td>1.90 2.44 3.22</td>
</tr>
<tr>
<td></td>
<td></td>
<td>below 0.10 eV</td>
<td>3.59</td>
<td>1.10 1.67 2.20</td>
</tr>
<tr>
<td>PU242</td>
<td>CAPT</td>
<td>4.0-0.54 eV</td>
<td>3.78</td>
<td>2.55 3.07 3.78</td>
</tr>
<tr>
<td>AM241</td>
<td>CAPT</td>
<td>4.0-0.54 eV</td>
<td><strong>5.54</strong></td>
<td>1.79 2.56 4.38</td>
</tr>
<tr>
<td></td>
<td></td>
<td>below 0.10 eV</td>
<td>1.80</td>
<td>1.01 1.69 1.80</td>
</tr>
</tbody>
</table>

**Data requirements:**

i) to improve $\sigma_{\text{fiss}}^{\text{Pu241}}$ below $\sim 400$ eV

ii) very tight $\sigma_{\text{cap}}$ requirements for Pu$^{241}$, Pu$^{240}$ and Pu$^{239}$ below $\sim 0.5$ eV

iii) in the resonance energy range, $\sigma_{\text{cap}}^{\text{U238}}$ from 24.8 to 9.12 keV

iv) for $\sigma_{\text{cap}}^{\text{Am241}}$ below $\sim 4$ eV
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CONCLUSIONS

1) Criticality calculations and inventory predictions were performed for the Phase-VII Benchmark using JEFF-3.1.1 nuclear data and computer programs ACAB and MCNP.

A set of additional calculations have been carried out using:
   i) Other nuclear decay data libraries (ORIGEN-S and ORIGEN-2.2)
   ii) Different neutron transport library (ENDF/B-VI)
   iii) Different computing tools (SCALE/KENO-VI)

We conclude that:
   i) Different decay data libraries have a negligible effect in $k_{\text{eff}}$ prediction
   ii) By contrary, neutron transport libraries have a very important effect

2) $k_{\text{eff}}$ sensitivity profiles of composition and multigroup cross-sections have been calculated with MCNP (PERT option)

3) Global uncertainty assessment
   i) Uncertainties in JEFF-3.1.1 Decay Data Library: negligible in $k_{\text{eff}}$ calculations
   ii) Uncertainties in cross-section data libraries from BOLNA (only variance values): $\Delta k_{\text{eff}} \sim 300-200$ pcm
   iii) Covariance information could increase these values

4) Cross section uncertainty and target assessment
   i) Corroborating the main data requirements for thermal systems pointed out by the OECD/NEA group of experts
   ii) We have added the $\sigma_{\text{cap}}^{\text{Am}^{241}}$ below $\sim 4$ eV (importance in the reactivity of Am$^{241}$ at $\sim 100$ y. of cooling time)