IMPACT OF THE FISSION YIELD COVARIANCE DATA IN BURN-UP CALCULATIONS

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   1.2 Propagation of FY Uncertainties in “pin-cell burn-up Benchmark”
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Summary and conclusions
“In nuclear criticality safety studies involving spent fuel, **burn-up credit** is being pursued and has been implemented in many countries as a means of more accurately and realistically determining the system reactivity by taking into account a decrease in the reactivity of spent fuel during irradiation”.


**Expert Group on Assay Data of Spent Nuclear Fuel (EGADSNF)**

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### Table 1. Commonly measured Fission Products of importance to different safety-related fuel applications.

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>Half-life (years)</th>
<th>Burn-up credit</th>
<th>Radiological safety</th>
<th>Waste management</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{79}$Se</td>
<td>$2.95 \times 10^{5}$</td>
<td></td>
<td></td>
<td></td>
<td>Metallic</td>
</tr>
<tr>
<td>$^{95}$Mo</td>
<td>Stable</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{96}$Sr</td>
<td>28.9</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{99}$Tc</td>
<td>$2.111 \times 10^{5}$</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>$^{101}$Ru</td>
<td>Stable</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{108}$Ru</td>
<td>371.6 days</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{103}$Rh</td>
<td>Stable</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{108}$Ag</td>
<td>Stable</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{125}$Sb</td>
<td>2.7586</td>
<td></td>
<td></td>
<td></td>
<td>Metallic</td>
</tr>
<tr>
<td>$^{129}$I</td>
<td>$1.6 \times 10^{7}$</td>
<td></td>
<td></td>
<td></td>
<td>Off gas during dissolution</td>
</tr>
<tr>
<td>$^{133}$Cs</td>
<td>Stable</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
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<td>2.065</td>
<td></td>
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<td></td>
</tr>
<tr>
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<td>$^{139}$La</td>
<td>Stable</td>
<td></td>
<td></td>
<td></td>
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<td>$^{143}$Nd</td>
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<td></td>
</tr>
<tr>
<td>$^{148}$Nd</td>
<td>Stable</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{144}$Ce</td>
<td>284.9 days</td>
<td></td>
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<td></td>
<td></td>
</tr>
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<td>$^{147}$Pm</td>
<td>2.623</td>
<td></td>
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</tr>
<tr>
<td>$^{147}$Sm</td>
<td>$1.06 \times 10^{11}$</td>
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<td></td>
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<tr>
<td>$^{148}$Sm</td>
<td>Stable</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{155}$Sm</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{151}$Sm</td>
<td>90</td>
<td></td>
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<td></td>
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<tr>
<td>$^{152}$Sm</td>
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<td></td>
<td></td>
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</tr>
<tr>
<td>$^{151}$Eu</td>
<td>Stable</td>
<td></td>
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<tr>
<td>$^{153}$Eu</td>
<td>Stable</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{154}$Eu</td>
<td>8.59</td>
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</tr>
<tr>
<td>$^{155}$Eu</td>
<td>4.753</td>
<td></td>
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<tr>
<td>$^{156}$Gd</td>
<td>Stable</td>
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### Table A.10: Hot Full Power (HFP) conditions for fuel pin-cell test problem

<table>
<thead>
<tr>
<th>Parameter</th>
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<tbody>
<tr>
<td>Fuel temperature (K)</td>
<td>900.0</td>
</tr>
<tr>
<td>Cladding Temperature (K)</td>
<td>600.0</td>
</tr>
<tr>
<td>Moderator (coolant) temperature (K)</td>
<td>562.0</td>
</tr>
<tr>
<td>Moderator (coolant) density (g/cm³)</td>
<td>0.7484</td>
</tr>
<tr>
<td>Reactor Power (MWt)</td>
<td>2772.0</td>
</tr>
<tr>
<td>Total number of fuel assemblies in the reactor core</td>
<td>177</td>
</tr>
<tr>
<td>Number of fuel rods per fuel assembly</td>
<td>208</td>
</tr>
<tr>
<td>Active core length (mm)</td>
<td>3571.20</td>
</tr>
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</table>

### Table A11: Configuration of pin-cell test problem

<table>
<thead>
<tr>
<th>Parameter</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Unit cell pitch (mm)</td>
<td>14.427</td>
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<tr>
<td>Fuel pellet diameter (mm)</td>
<td>9.391</td>
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<tr>
<td>Fuel pellet material</td>
<td>UO2</td>
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<tr>
<td>Fuel density (g/cm³)</td>
<td>10.283</td>
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<tr>
<td>Fuel enrichment (w/o)</td>
<td>4.85</td>
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<tr>
<td>Cladding outside diameter (mm)</td>
<td>10.928</td>
</tr>
<tr>
<td>Cladding thickness (mm)</td>
<td>0.673</td>
</tr>
<tr>
<td>Cladding material</td>
<td>Zircaloy-4</td>
</tr>
<tr>
<td>Cladding density (g/cm³)</td>
<td>6.55</td>
</tr>
<tr>
<td>Gap material</td>
<td>He</td>
</tr>
<tr>
<td>Moderator material</td>
<td>H2O</td>
</tr>
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</table>

### Table A12: Simplified operating history data for benchmark problem pin-cell calculation and specific power

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>Operating cycle</td>
<td>1</td>
</tr>
<tr>
<td>Burn time (days)</td>
<td>1825.0</td>
</tr>
<tr>
<td>Final Burnup (GWd/MTU)</td>
<td>61.28</td>
</tr>
<tr>
<td>Downtime (days)</td>
<td>1870.0</td>
</tr>
<tr>
<td>Specific power (kW/kgU)</td>
<td>33.58</td>
</tr>
</tbody>
</table>

Expert Group on “Uncertainty Analysis in Modelling”
1.2 Propagation of FY Uncertainties in “pin-cell burn-up Benchmark”

- References on FY uncertainty calculations:
    - Implemented in XSUSA Methodology (Monte Carlo) using FY-ENDF/B-VII.1

<table>
<thead>
<tr>
<th></th>
<th>0 GWD/MTU mean</th>
<th>0 GWD/MTU rel. std. dev.</th>
<th>10 GWD/MTU mean</th>
<th>10 GWD/MTU rel. std. dev.</th>
<th>30 GWD/MTU mean</th>
<th>30 GWD/MTU rel. std. dev.</th>
<th>60 GWD/MTU mean</th>
<th>60 GWD/MTU rel. std. dev.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ΔXS</td>
<td>ΔDD</td>
<td>ΔFYs</td>
<td>ΔXS</td>
<td>ΔDD</td>
<td>ΔFYs</td>
<td>ΔXS</td>
<td>ΔDD</td>
</tr>
<tr>
<td>Nd-148</td>
<td>GRS</td>
<td>0.00E+00</td>
<td>1.76E-06</td>
<td>0.3</td>
<td>0.0</td>
<td>16.5</td>
<td>5.58E-06</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Table 2. Cumulative fission yield uncertainty value by fission in $^{235}$U and $^{239}$Pu with thermal neutrons. Data processed from ENDF/B-VII.1 Fission Yield Data Library.

<table>
<thead>
<tr>
<th>CFY: Rel. err. (in%)</th>
<th>By neutron thermal fission in:</th>
<th>CFY: Rel. err. (in%)</th>
<th>By neutron thermal fission in:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$^{235}$U</td>
<td>$^{239}$Pu</td>
<td>$^{235}$U</td>
</tr>
<tr>
<td>$^{148}$Nd</td>
<td>0.35</td>
<td>0.50</td>
<td>1.0</td>
</tr>
<tr>
<td>$^{137}$Cs</td>
<td>0.50</td>
<td>0.50</td>
<td>64.0</td>
</tr>
<tr>
<td>$^{139}$La</td>
<td>0.70</td>
<td>2.80</td>
<td>-</td>
</tr>
<tr>
<td>$^{129}$I</td>
<td>-</td>
<td>-</td>
<td>64.0</td>
</tr>
<tr>
<td>$^{109}$Ag</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Justification of FY covariance generation methodologies

\[
\begin{align*}
\frac{dN_7(t)}{dt} &= (-\lambda_7 - \sigma_c^2 \Phi) N_7 + \Sigma_f \Phi \cdot y_{7 \text{cum}}^2 \\
\frac{dN_8(t)}{dt} &= -\sigma_c^3 \phi N_8 + \sigma_c^2 \phi N_7 + \Sigma_f \Phi \cdot y_{8 \text{cum}}^2 \\
N_8(t) &\approx \frac{\Sigma_f \Phi \cdot y_{8 \text{cum}}^2}{\sigma_c^3 \phi} (1 - e^{-\sigma_c^2 \Phi t})
\end{align*}
\]

\[
\frac{\Delta N_8}{N_8} \approx \frac{\Delta y_{8 \text{cum}}^2}{y_{8 \text{cum}}^2} < 1\%
\]
Fission yield covariance generation and uncertainty propagation through fission pulse decay heat calculation

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\textsuperscript{b}ULB, Université Libre de Bruxelles, Avenue Franklin Roosevelt 50, 1050 Bruxelles, Belgium
\textsuperscript{c}Dpto. de Ingeniería Nuclear, Escuela Técnica Superior de Ingenieros Industriales, Universidad Politécnica de Madrid UPM, José Gutiérrez Abascal 2, 28006 Madrid, Spain
\textsuperscript{d}Instituto de Fusión Nuclear, Escuela Técnica Superior de Ingenieros Industriales, Universidad Politécnica de Madrid UPM, José Gutiérrez Abascal 2, 28006 Madrid, Spain

\textbf{ARTICLE INFO}

\textbf{ABSTRACT}

Fission product yields are fundamental parameters in burnup/activation calculations and the impact of their uncertainties was widely studied in the past. Evaluations of these uncertainties were released, still without covariance data. Therefore, the nuclear community expressed the need of full fission yield covariance matrices to be able to produce inventory calculation results that take into account the complete uncertainty data.

State-of-the-art fission yield data and methodologies for fission yield covariance generation were researched in this work. Covariance matrices were generated and compared to the original data stored in the library. Then, we focused on the effect of fission yield covariance information on fission pulse decay heat results for thermal fission of \textsuperscript{233}U. Calculations were carried out using different libraries and codes (ACAB and ALEPH-2) after introducing the new covariance values. Results were compared with those obtained with the uncertainty data currently provided by the libraries. The uncertainty quantification was performed first with Monte Carlo sampling and then compared with linear perturbation. Indeed, correlations between fission yields strongly affect the uncertainty of decay heat. Eventually, a sensitivity analysis of fission product yields to fission pulse decay heat was performed in order to provide a full set of the most sensitive nuclides for such a calculation.

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FY covariance data generation:

- Great efforts have been committed to develop methodologies for correlation generation (full covariance matrices) for FY data.
- This task is in the scope of the framework of WPEC-SG37.

Methodologies proposed at the kick-off meeting of WPEC-SG37 (May 2013), based on:

- **Perturbation theory** applied to the “Five Gaussians and Wahl’s models” (Musgrove et al., 1973; Wahl, 1988), proposed by Pigni et al. (2013).

- **Monte Carlo parameter perturbation** using the GEF code (Schmidt and Jurado, 2010), presented by Schmidt (2013).

- **Bayesian/general least-squares (GLS) method**, where the IFY covariance matrix is updated with information on the chain yields as proposed by Kawano and Chadwick (2013), and previously applied by Katakura (2012).
  - A variation of this proposal, with IFYs covariance matrix updated with CFYs ones is described and reported by UPM/SCK (L. Fiorito et al., 2014)
The updating process is represented by Eqs. (11) and (12),

\[
\begin{align*}
\theta - \theta_a & = V_a S' (SV_a S' + V)^{-1} (\eta - y_a) \\
V_s & = V_a - V_a S' (SV_a S' + V)^{-1} S V_a
\end{align*}
\] (11) (12)

where \(V_a\) is the variance matrix of prior estimates of the parameters \((\theta_a)\), \(V\) is the variance matrix of the introduced data fitting the constraining system \((\eta)\), and \(V_s\) is the updated covariance matrix of the system parameters \((\theta)\). Superscript \(t\) refers to the transpose of a matrix.

Simple equations to generate the updated covariance matrix for IFYs can be derived from Eq. (12), resulting in Eqs. (13) and (14) which represent the diagonal and off-diagonal terms respectively:

\[
\begin{align*}
\mu_{ii} & = \sigma_i^2 \left( 1 - \frac{\sigma_i^2}{\sigma^2 + \sum_j \sigma_j^2} \right) \\
\mu_{ij} & = -\frac{\sigma_i^2 \sigma_j^2}{\sigma^2 + \sum_j \sigma_j^2}
\end{align*}
\] (13) (14)

Here, \(\sigma_i\) is the standard deviation of the \(i\)th IFY and \(\sigma\) is the standard deviation of evaluated MFY. Sum \(\sum_j \sigma_j^2\) includes all the isotopes in the same mass chain as it relates MFYs to IFYs.

## 2. Methodology to propagate ND Uncertainties

### Monte Carlo burnup calculation SCALE6.1.2/TRITON

- Generation of a set of 1000 FY random libraries for U\textsuperscript{235} and Pu\textsuperscript{239}

<table>
<thead>
<tr>
<th>“No-correlation”. FY uncertainty is the standard deviation of ENDF/B-VII.1</th>
<th>“Correlation” matrix using Katakura methodology</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_U = \begin{bmatrix} \left( \frac{\Delta Y_1}{Y_1} \right)^2 &amp; 0 &amp; 0 \ 0 &amp; \ddots &amp; 0 \ 0 &amp; 0 &amp; \left( \frac{\Delta Y_K}{Y_K} \right)^2 \end{bmatrix}$</td>
<td>$V_U = \begin{bmatrix} \left( \frac{\Delta Y_1}{Y_1} \right)^2 &amp; \text{cov}(Y_1,Y_2)/Y_1Y_2 &amp; \cdots &amp; \text{cov}(Y_1,Y_K)/Y_1Y_K \ \text{cov}(Y_K,Y_1)/Y_KY_1 &amp; \ddots &amp; \cdots &amp; \vdots \ \vdots &amp; \cdots &amp; \left( \frac{\Delta Y_K}{Y_K} \right)^2 \end{bmatrix}$</td>
</tr>
</tbody>
</table>

- PDF: Normal distribution, with “zero” for negative values.

### Sensitivity/Uncertainty calculation SCALE6.1.2/TRITON

- Calculation of Sensitivity coefficients: $S_{FYi,j}^U = (\Delta N_i/N_i) / (\Delta FY_{i,j}^U/FY_{i,j})$
- S/U: 1\textsuperscript{st} Order Approximation, “Sandwinch Formula”

$$\frac{\text{var}(N_i)}{N_i^2} = (S_{FY1}^{U235} S_{FY1}^{Pu239} \cdots) \left[ \begin{bmatrix} V_{U235} & 0 \\ \vdots & \ddots \end{bmatrix} \begin{bmatrix} V_{Pu239} & 0 \\ \vdots & \ddots \end{bmatrix} \right] \left( \begin{bmatrix} S_{FY1}^{U235} \\ \vdots \end{bmatrix} \right)$$
### 2.1 Monte Carlo Methodology: “Number Density Uncertainty”

Table 3. Uncertainty in number density (in %) for some important fission products at 60 GWd/MTU. Fission Yield source of uncertainty (standard deviation) is taken from ENDF/B-VII.1.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{79}$Se</td>
<td>3.5</td>
<td>16.0</td>
<td>-</td>
<td>$^{142}$Nd</td>
<td>0.8</td>
<td>3.5</td>
<td>-</td>
</tr>
<tr>
<td>$^{90}$Sr</td>
<td>0.8</td>
<td>6.2</td>
<td>-</td>
<td>$^{143}$Nd</td>
<td>0.4</td>
<td>6.5</td>
<td>5.9</td>
</tr>
<tr>
<td>$^{95}$Mo</td>
<td>0.5</td>
<td>8.4</td>
<td>7.9</td>
<td>$^{144}$Nd</td>
<td>0.2</td>
<td>3.9</td>
<td>-</td>
</tr>
<tr>
<td>$^{99}$Tc</td>
<td>0.8</td>
<td>10.0</td>
<td>9.5</td>
<td>$^{145}$Nd</td>
<td>0.4</td>
<td>7.1</td>
<td>6.7</td>
</tr>
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<td>$^{101}$Ru</td>
<td>0.7</td>
<td>4.6</td>
<td>-</td>
<td>$^{146}$Nd</td>
<td>0.7</td>
<td>10.8</td>
<td>-</td>
</tr>
<tr>
<td>$^{106}$Ru</td>
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<td>-</td>
<td>$^{147}$Nd</td>
<td>0.8</td>
<td>13.7</td>
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<td>12.1</td>
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<td>10.3</td>
<td>-</td>
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<td>17.8</td>
<td>-</td>
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<td>10.6</td>
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<td>$^{129}$I</td>
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<td>-</td>
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<td>$^{131}$Xe</td>
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<td>6.9</td>
<td>-</td>
<td>$^{151}$Sm</td>
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<td>11.7</td>
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<td>$^{135}$Xe</td>
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<td>5.1</td>
<td>-</td>
<td>$^{152}$Sm</td>
<td>0.6</td>
<td>11.3</td>
<td>8.8</td>
</tr>
<tr>
<td>$^{133}$Cs</td>
<td>0.3</td>
<td>3.4</td>
<td>1.7</td>
<td>$^{151}$Eu</td>
<td>0.7</td>
<td>12.1</td>
<td>-</td>
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<tr>
<td>$^{134}$Cs</td>
<td>0.3</td>
<td>3.0</td>
<td>-</td>
<td>$^{153}$Eu</td>
<td>0.8</td>
<td>9.9</td>
<td>-</td>
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<tr>
<td>$^{135}$Cs</td>
<td>0.3</td>
<td>3.4</td>
<td>-</td>
<td>$^{154}$Eu</td>
<td>0.8</td>
<td>10.4</td>
<td>-</td>
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<tr>
<td>$^{137}$Cs</td>
<td>0.5</td>
<td>1.5</td>
<td>1.7</td>
<td>$^{155}$Gd</td>
<td>1.0</td>
<td>10.5</td>
<td>8.8</td>
</tr>
<tr>
<td>$^{139}$La</td>
<td>0.9</td>
<td>3.2</td>
<td>-</td>
<td>$^{156}$Gd</td>
<td>1.2</td>
<td>9.0</td>
<td>-</td>
</tr>
<tr>
<td>$^{144}$Ce</td>
<td>0.2</td>
<td>8.0</td>
<td>-</td>
<td>$^{157}$Gd</td>
<td>1.3</td>
<td>9.5</td>
<td>-</td>
</tr>
<tr>
<td>$^{158}$Gd</td>
<td>2.3</td>
<td>11.3</td>
<td>-</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

i) No correlation between fission products (ΔFYs/No corr.)

ii) FYs including correlations for $^{235}$U and $^{239}$Pu taken from Katakura methodology (ΔFYs/Corr.)

iii) GRS calculation
2.1.1 Monte Carlo Methodology: “Number Density Uncertainty” for $^{148}$Nd, $^{137}$Cs and $^{139}$La

**Figure 1.** Relative standard deviations (in %) of $^{148}$Nd, $^{137}$Cs and $^{139}$La (burnup indicators). Calculations performed with SCALE6.1.2, a set of 1000 random fission yield libraries based on ENDF/B-VII.1.

- **i)** “No corr.” case, no-correlation between FYs
- **ii)** “Corr.” case where fission yield correlation matrices supplied for $^{235}$U and $^{239}$Pu using Katakura methodology.
2.1.2 Monte Carlo Methodology: “Number Density Uncertainty” for $^{109}\text{Ag}$ and $^{129}\text{I}$

Figure 2. Relative standard deviations (in %) of $^{109}\text{Ag}$ (burn-up credit) and $^{129}\text{I}$ (waste management). Calculations performed with SCALE6.1.2, a set of 1000 random fission yield libraries based on ENDF/B-VII.1.

i) “No corr.” case, no-correlation between FYs

ii) “Corr.” case where fission yield correlation matrices supplied for $^{235}\text{U}$ and $^{239}\text{Pu}$ using Katakura methodology.

WHY?
2.1.3 Low correction for $^{109}$Ag using Katakuria correlation matrix

Mass Yield Data

Table 4. Range of mass chain yield uncertainties (in %) reported by England (1993) by fission in $^{235}$U and $^{239}$Pu with thermal neutrons.


<table>
<thead>
<tr>
<th>A mass</th>
<th>$^{235}$U</th>
<th>$^{239}$Pu</th>
<th>A mass</th>
<th>$^{235}$U</th>
<th>$^{239}$Pu</th>
</tr>
</thead>
<tbody>
<tr>
<td>109</td>
<td>4-6</td>
<td>2.8-4</td>
<td>137</td>
<td>0.35-0.5</td>
<td>0.35-0.5</td>
</tr>
<tr>
<td>129</td>
<td>0.7-1.0</td>
<td>2-2.8</td>
<td>139</td>
<td>0.5-0.7</td>
<td>2-2.8</td>
</tr>
<tr>
<td>148</td>
<td>-</td>
<td>-</td>
<td>148</td>
<td>&lt;0.35</td>
<td>.35-0.5</td>
</tr>
</tbody>
</table>

Mass Yield Data

\[
\mu_{ii} = \sigma_i^2 \left( 1 - \frac{\sigma_i^2}{\sigma^2 + \sum_j \sigma_j^2} \right)
\]

\[
\mu_{ij} = \frac{\sigma_i^2 \sigma_j^2}{\sigma^2 + \sum_j \sigma_j^2}
\]

Here, $\sigma_i$ is the standard deviation of the $i$th IFY and $\sigma$ is the standard deviation of evaluated MFY. Sum $\sum_j \sigma_j^2$ includes all the isotopes in the same mass chain as it relates MFYs to IFYs.

Deficiencies for $^{109}$Ag:

- High value of MFY “standard deviation”
- Only takes into account correction for IFY for the same “A”
  (exception for Ru108)
2.2 S/U Methodology:
“Number Density Uncertainty”

**Calculation of Sensitivity Coefficients:**

\[ S_{FY,ij}^U = \frac{(\Delta N_i/N_i)}{(\Delta FY_{ij}/FY_{ij})} \]

Figure 3. Sensitivity \( Nd^{148} \) coefficients calculated with SCALE6.1.2/TRITON by a linear perturbation of the IFY values (sensitivities with values higher that 0.05 are shown)
2.2.1 S/U Methodology: \( ^{148}\text{Nd},^{139}\text{La} \) and \( ^{137}\text{Cs} \) (burnup indicators)

Table 5. Uncertainty of the main independent fission yield contributors to the generation of \( ^{137}\text{Cs},^{137}\text{La} \) and \( ^{148}\text{Nd} \) by fission in \( ^{235}\text{U} \) and \( ^{239}\text{Pu} \) with thermal neutrons. Data processed from ENDF/B-VII.1 Fission Yield Data Library.

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>137Cs by fission in:</th>
<th>139La by fission in:</th>
<th>148Nd by fission in:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( ^{235}\text{U} )</td>
<td>( ^{239}\text{Pu} )</td>
<td>( ^{235}\text{U} )</td>
</tr>
<tr>
<td>137Te</td>
<td>8.0</td>
<td>64.0</td>
<td>64.0</td>
</tr>
<tr>
<td>137I</td>
<td>4.0</td>
<td>6.0</td>
<td>23.0</td>
</tr>
<tr>
<td>137Xe</td>
<td>2.8</td>
<td>4.0</td>
<td>-</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>139I</td>
<td>8.0</td>
<td>23.0</td>
<td>64.0</td>
</tr>
<tr>
<td>139Xe</td>
<td>2.0</td>
<td>4.0</td>
<td>45.0</td>
</tr>
<tr>
<td>139Cs</td>
<td>4.0</td>
<td>23.0</td>
<td>64.0</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

S/U, Applying “Sandwich Formula”:

\[
\frac{\text{var}(N_i)}{N_i^2} = (SU_{235}^{FYI} \quad SP_{239}^{FYI} \quad \ldots) \begin{bmatrix} V_{U235} & 0 & 0 \\ 0 & V_{Pu239} & 0 \\ 0 & 0 & \ddots \end{bmatrix} \begin{bmatrix} SU_{235}^{FYI} \\ SP_{239}^{FYI} \\ \vdots \end{bmatrix}
\]

Table 6. Comparison of S/U and Monte Carlo uncertainty prediction at 60 GWD/TMU. FY uncertainty with “No corr.”

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>S/U</th>
<th>Monte Carlo</th>
</tr>
</thead>
<tbody>
<tr>
<td>148Nd</td>
<td>14.2</td>
<td>13.7</td>
</tr>
<tr>
<td>137Cs</td>
<td>1.50</td>
<td>1.50</td>
</tr>
<tr>
<td>139La</td>
<td>3.20</td>
<td>3.20</td>
</tr>
</tbody>
</table>
2.2.2 S/U Methodology: $^{109}$Ag and $^{129}$I

Calculation of Sensitivity Coefficients:

$$S_{FY_{i,j}}^{U} = \frac{\Delta N_i/N_i}{\Delta FY_{i,j}^{U}} / FY_{i,j}^{U}$$

Figure 4. Sensitivity Ag$^{109}$ coefficients calculated with SCALE6.1.2/TRITON by a linear perturbation of the IFY values (sensitivities with values higher that 0.05 are shown)
2.2.2 S/U Methodology: $^{109}\text{Ag}$ and $^{129}\text{I}$

Table 7. Uncertainty of the main independent fission yield contributors to the generation of $^{109}\text{Ag}$ and $^{129}\text{I}$ by fission in $^{235}\text{U}$ and $^{239}\text{Pu}$ with thermal neutrons. Data processed from ENDF/B-VII.1 Fission Yield Data Library.

<table>
<thead>
<tr>
<th>IFY: Rel. err. (in%)</th>
<th>Generation of $^{109}\text{Ag}$ by fission in:</th>
<th>IFY: Rel. err. (in%)</th>
<th>Generation of $^{129}\text{I}$ by fission in:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$^{235}\text{U}$</td>
<td>$^{239}\text{Pu}$</td>
<td>$^{235}\text{U}$</td>
</tr>
<tr>
<td>$^{109}\text{Mo}$</td>
<td>64.0</td>
<td>64.0</td>
<td>$^{129}\text{Mn}$</td>
</tr>
<tr>
<td>$^{109}\text{Tc}$</td>
<td>64.0</td>
<td>64.0</td>
<td>$^{129}\text{Sn}$</td>
</tr>
<tr>
<td>$^{109}\text{Ru}$</td>
<td>64.0</td>
<td>64.0</td>
<td>$^{129}\text{Sb}$</td>
</tr>
<tr>
<td>$^{108}\text{Ru}$</td>
<td>64.0</td>
<td>64.0</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 8. Comparison of S/U and Monte Carlo uncertainty prediction at 60 GWd/TMU. FY uncertainty with “No corr.”

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>S/U</th>
<th>Monte Carlo</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{109}\text{Ag}$</td>
<td>25.0</td>
<td>17.8</td>
</tr>
<tr>
<td>$^{129}\text{I}$</td>
<td>20.3</td>
<td>20.7</td>
</tr>
</tbody>
</table>

- Our Monte Carlo method uses a “truncated Normal PDF”. Then, the new random set yields a reduced uncertainty.

WHY?

Our Monte Carlo method uses a “truncated Normal PDF”. Then, the new random set yields a reduced uncertainty.
Figure 5. Relative standard deviation in $k_{\text{eff}}$ (in %):

i) SCALE/XSUSA calculation performed by GRS [7] only uncertainties in cross-section data,

ii) SCALE/TSUNAMI calculation [2] only uncertainties in cross-section data,

iii) SCALE/XUSA calculation by GRS with uncertainties only in fission yield data taken from ENDF/B-VII.1/FY data library,

iv) Monte Carlo with a set of 1000 different fission yield data libraries based on ENDF/B-VII.1 with no-correlation between fission yields (“No corr.”)

v) Monte Carlo with correlations generated by Katakura method in $^{235}\text{U}$ and $^{239}\text{Pu}$ (“Corr.”).
Summary and conclusions

- The present study has demonstrated the importance of covariance terms if fission yield data libraries to improve estimations of uncertainties in burn-up applications.

- Results in a LWR pin-cell burnup benchmark.

- It has been proved that non-correlated independent fission yields data bring to overestimated uncertainties in the number density and criticality predictions.

- Comparison between S/U and Monte Carlo shows good agreement (except for $^{109}\text{Ag}$).

- Assessment of the methodology to generate fission yield covariance data based on Katakura model using information of experimental mass fission yield data:
  - Covariance fission yield data for $^{235}\text{U}$ and $^{239}\text{Pu}$ fissile nuclides were processed.
  - Covariance for isotopes in the same mass chain are modified.
  - Covariance data (by Katakura) changes the criticality and number density uncertainties, reducing its variance to almost a negligible effect (except for $^{109}\text{Ag}$).
Acknowledgements

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