PROPAGATION OF NUCLEAR DATA UNCERTAINTIES IN FUEL CYCLE CALCULATIONS USING MONTE-CARLO TECHNIQUE

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Abstract

The uncertainty propagation in fuel cycle calculations due to Nuclear Data (ND) is an important issue for:

- Present fuel cycles (e.g. high burnup fuel programme)
- New fuel cycles designs (e.g. fast breeder reactors and ADS)

Different error propagation techniques can be used:

- Sensitivity analysis
- Response Surface Method
- Monte Carlo technique

Then, in this paper, it is assessed the impact of ND uncertainties on the decay heat and radiotoxicity in two applications:

- Fission Pulse Decay Heat calculation (FPDH)
- Conceptual design of European Facility for Industrial Transmutation (EFIT)

The complete set of uncertainty data for cross sections (EAF2007/UN), decay data and fission yield data (JEFF-3.1.1) are processed and used in ACAB code.
PART I: Methodology to propagate ND uncertainties using Monte Carlo technique

PART II: Application of Monte Carlo technique

A. Fission Pulse Decay Heat calculation

B. EFIT fuel cycle calculation

CONCLUSIONS
Goal: “To analyse how ND uncertainties are transmitted to response functions”

\[
\frac{dN}{dt} = [\lambda]N + [\sigma_{\text{eff}}] \cdot \Phi N + [(\gamma \sigma_{\text{fiss}})_{\text{eff}}] \cdot \Phi N = A \cdot N \quad \Rightarrow \quad N_i = N_i(\lambda, \sigma, \gamma)
\]

1) Sensitivity / Uncertainty Analysis (S/U)
   - First order Taylor series (linear approximation)

2) Monte Carlo Uncertainty Analysis (MC)
   - To treat the global effect of all nuclear data uncertainties
   - Without any approximation
PART I
Methodology to propagate ND uncertainties

Monte Carlo technique

- Individual / All together sampling $(\lambda, \sigma, \gamma)$
- PDFs

1. Normal distribution
   $$\sigma_j \rightarrow N[\sigma_{j0}, DST(\sigma_j)] \Rightarrow \varepsilon_j \rightarrow N(0, \Delta_j)$$
   $$\Rightarrow \text{If } \Delta_j \uparrow \uparrow \Rightarrow \text{Maybe } \sigma_j < 0$$

2. LogNormal distribution
   $$\log\begin{pmatrix} (\sigma_1 / \sigma_{10}) \\ \vdots \\ (\sigma_m / \sigma_{m0}) \end{pmatrix} \rightarrow N(0, M)$$

Nuclear Data libraries Collapsed
Mean Values $\lambda, \gamma, \sigma$
Uncertainties (Standard Desv)

Samplig
\[ \lambda_1, \gamma_1, \sigma_1 \]
\[ \lambda_2, \gamma_2, \sigma_2 \]
... 
\[ \lambda_n, \gamma_n, \sigma_n \]

ACAB

Results
\[ N_1 \]
\[ N_2 \]
... 
\[ N_n \]
PART I

Methodology to propagate ND uncertainties

Uncertainty data

- Cross section from activation-oriented nuclear data libraries

  EAF2007-UN

  \[ W_{180}^{n,\gamma} \]

  e.g.:

  \[ W_{180}^{n,\gamma} \]

  \[ E_i (eV) \]

  \[ \Delta^2_{I=1,EAF} \ (\text{relative error, } \Delta) \sim \Delta_{I=1,EXP} = \Delta_{I=1,EAF}/3 \]

- Fission yield from evaluated nuclear data library

  JEFF 3.1.1

  \[ \gamma_{Th232\rightarrow H3,400KeV} + 1\sigma_{\gamma} \]
PART I
Methodology to propagate ND uncertainties

Processing and collapsing of nuclear data

Collapsing method:

- Cross section: Conservation of reaction rate

\[
\text{Rate}_{j \rightarrow i} = \int_E \sigma_{j \rightarrow i}(E) \cdot \phi(E) \cdot dE = \sigma^\text{eff}_{j \rightarrow i} \cdot \phi_T
\]

- Uncertainties: Using **Sandwich rule** (*Propagation of Momentum, first order*)

\[
\Delta^2 = \omega^T V \omega
\]

Processing and collapsing of nuclear data

→ Cross section

Given \( V \) the G-by-G variance matrix of the relative cross sections vector, the variance \( \Delta^2 \) of the relative spectrum-averaged cross section is:

\[
\Delta^2 = \omega^T V \omega
\]

with

\[
\omega = \left[ \frac{\phi_1}{\phi \sigma_{\text{eff}}} , \ldots , \frac{\phi_G}{\phi \sigma_{\text{eff}}} \right]^T
\]

\[
\bar{\phi} = \phi_1 + \phi_2 + \cdots + \phi_G
\]

\[
\sigma_{\text{eff}} = \frac{\phi_1 \sigma_1 + \phi_2 \sigma_2 + \cdots + \phi_G \sigma_G}{\phi_1 + \phi_2 + \cdots + \phi_G}
\]

→ Fission yield

Given \( G \) the M-by-M variance matrix of the relative fission yield vector, the variance \( \Delta^2 \) of the relative spectrum-averaged fission yield is:

\[
\Delta^2 = \omega^T G \omega
\]

with

\[
\omega = \left[ \frac{\gamma_{1,\text{fiss}}^j}{\phi \sigma_{\text{fiss}}} , \ldots , \frac{\gamma_{G,\text{fiss}}^j}{\phi \sigma_{\text{fiss}}} \right]^T
\]

where

\[
\gamma_{j,i}^\text{eff} = \gamma_{1,\text{fiss}}^j \frac{\phi_1}{\phi_1 + \cdots + \phi_G} + \gamma_{G,\text{fiss}}^j \frac{\phi_G}{\phi_1 + \cdots + \phi_G}
\]
Advantages & Disadvantages of Monte Carlo Technique

**Advantages**
- Collapsing to one energy group → Reduce amount of variables to sample
- No sensitivity coefficients should be calculated
- No approximation on equations → Take into account non-linear effects

**Disadvantages**
- How to check if the phase space is well sampled?
- Which PDFs should be taken?
- Computational demanding
APPLICATIONS:

A. Fission Pulse Decay Heat calculation

B. EFIT fuel cycle calculation
A. Fission Pulse Decay Heat calculation
PART II

A. Fission Pulse Decay Heat calculation

Description of the problem

- Decay heat of a single thermal fission event in Pu239
- Isotopes: only Fission Products (FPs)
- Only Fission yield (FY) and Decay data (Energy/Decay constant) uncertainties are propagated

\[ DH_x = \lambda_x \cdot N_x \cdot E_x \]

\[ \text{FPs} \]

\[ 97 \text{Sr}_{38} \]

\[ 104 \text{mNb}_{41} \]

\[ 104 \text{Mo}_{42} \]

\[ DH_{\text{Nb104m}} \]

\[ DH_{\text{Mo104}} \]
PART II

A. Fission Pulse Decay Heat calculation

Calculations

- Histories launched/case: 300
- Relative error followed

Case studied

- Total decay heat
- Beta decay heat
- Gamma decay heat

Only known uncertainties  //  All with uncertainties

For unknown uncertainties

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<th>Decay Mode</th>
<th>Uncertainty</th>
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<td>Alfa</td>
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<tr>
<td>Beta</td>
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<tr>
<td>Gamma</td>
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Compared with:
- JEFF report 20
- Tobias exp. data
Total decay heat

![Graph showing cooling time vs. C/E ratio with positive bias indication]
B. EFIT fuel cycle calculation
Reference system

One of the preliminary conceptual designs of the **European Facility for Industrial Transmutation (EFIT)**

**Constant neutron environment:**
- neutron flux: $3.12 \times 10^{15} \text{ n/cm}^2 \text{ s}$
- average energy $<E> = 0.37 \text{ MeV}$

**Calculations for discharge burn-up:**
- 150 GWd/tHM (778 irradiation days)
- 500 GWd/tHM (3225 irradiation days)
PART II

B. EFIT fuel cycle calculation

Calculations

• Histories launched:
  1000/DH case
  300/RTX case

Case studied

1. Decay heat
2. Radiotoxicity
   a. Inhalation dose
   b. Ingestion dose

All uncertainties are propagated:

- Individually \( \sigma, \gamma, \lambda \)
- All together

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Decay heat for 150 GWd/tHM

Main contributors analysis

\[ DH_{total} = \sum_{i=\text{isotope}} DH_i \]

\[ \text{var}(y) = \sum_{i=1}^{N} \text{var}(y_i) + \sum_{i,j=1;i\neq j}^{N} \text{cov}(y_i, y_j) \]

\[ \sum_{i=1}^{N} \text{var}(y_i) \gg \sum_{i,j=1;i\neq j}^{N} \text{cov}(y_i, y_j) \]

\[ \sigma_x^2 = \sum_{i=1}^{N} \sigma_{y_i}^2 \cdot \frac{y_i^2}{x^2} = \sum_{i=1}^{N} \text{error}(y_i)^2 \cdot \frac{y_i^2}{x^2} \]
Decay heat for 150 GWd/tHM

Main contributors

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<thead>
<tr>
<th></th>
<th>Cm242</th>
<th>Cm244</th>
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Error (%)

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Cooling Time (years)

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PART II

B. EFIT fuel cycle calculation

Radiotoxicity for 150 GWd/tHM

Ingestion

Due to FY / XS error

Xe133  Cm244  Pu238
Am241    Rn222
CONCLUSIONS
Monte Carlo technique for ND uncertainty propagation in activation calculations

- Pre-processing of nuclear data is needed:
  - Identifying uncertainties
  - Collapsing of nuclear data

- Implemented on ACAB code

Monte Carlo technique VS deterministic calculations / experimental data

- A good agreement is found between both

- A method to identify main contributors to error is developed based on MC results

- PDFs dependency is found in FPDH calculation, but not in EFIT calculation
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