Reaction rate uncertainty quantification and propagation, variance-covariance
• Single irradiation pulse followed by cooling
• Multiple irradiation pulses
  ▪ changing flux amplitude
  ▪ cooling
• Multi-step
  ▪ changing flux amplitude and spectrum
  ▪ changing cross-section (e.g., temperature dependence)
  ▪ cooling
• Pathways and sensitivity for all cases
• Extracts and reduces nuclear and radiological data
• Solves rate equations for time evolution of inventory
• Computes and outputs derived radiological quantities
• Identifies and quantifies key reactions and decay processes:
  • dominant nuclides
  • pathways and uncertainty
  • Monte-Carlo sensitivity and uncertainty
  • reduced model calculations
• Uncertainty calculation
  • input cross-section and decay uncertainties
  • output uncertainties for all radiological quantities
• Condense run extracts from decay files:
  ▪ decay constant $\lambda$
  ▪ decay constant uncertainty $\Delta \lambda$

• Collapse constructs flux spectrum weighted averages:

  ➢ Library input
  • cross-section vs energy
  • covariances vs energy
  • flux spectrum vs energy

  $$W_i = \frac{\phi_i}{\sum_{i=1}^{N} \Phi_i}$$

  ➢ Data used in code
  • collapsed cross-section $\overline{XS}$
  • collapsed uncertainty $\Delta$
• reactions $X$ and $Y$
• energy bins $i$ and $j \in [1,N]$ with $N = 709$
• uses $\text{Cov}(X_i,Y_j)$ for $X \neq Y$ only in Monte-Carlo
• collapse $\text{Cov}(X_i,X_j)$ to get uncertainty $\Delta$ for $\bar{X}$

\[ \text{var} = \sum_{i=1}^{N} \sum_{j=1}^{N} W_i W_j \text{Cov}(X_i, X_j); \qquad \Delta = \{1|3\} \sqrt{\text{var}} / \bar{X} \]

• Collapse $\text{Cov}(X_i,Y_j)$ to get $\text{Cov}(\bar{X}, \bar{Y})$ for $X \neq Y$
• Cov data in ENDF file 33 & 40, NI type LB=1, 5, 6
• Cov data in wider energy bins $k \in [1, M]$, $M \sim 40$
The projection operator \( S_i^k \) maps cross-section energy bins to covariance energy bins:

\[
S_i^k = \begin{cases} 
1 & \text{bin } i \text{ in bin } k \\
0 & \text{otherwise}
\end{cases}
\]

The ENDF style covariance data forms, different LB’s are read directly without the need of pre-processing.
Using $S_i^k$, the formula to construct estimates of the covariance matrix are as follows:

\[
LB = 1: \quad Cov(X_i, X_j) = \sum_{k=1}^{M} S_i^k S_j^k F_k X_i X_j
\]

\[
LB = 5: \quad Cov(X_i, Y_j) = \sum_{k=1}^{M} \sum_{k' = 1}^{M'} S_i^k S_j^{k'} F_{kk'} X_i Y_j
\]

\[
LB = 6: \quad Cov(X_i, Y_j) = \sum_{k=1}^{M} \sum_{k' = 1}^{M'} S_i^k S_j^{k'} F_{kk'} X_i Y_j
\]

\[
LB = 8: \quad Cov(X_i, X_j) = \sum_{k=1}^{M} S_i^k S_j^k 1000F_k \quad (Koning)
\]

\[
(\text{or}) \quad = \sum_{k=1}^{M} S_i^k \delta_{ij} 1000F_k
\]

The LB=1 case is the one that was applied to the computation of $\Delta$ for the EAF’s libraries.
Given\{\overline{XS}, \lambda\}

- select irradiation scenario
- solve for radiological quantities

Use \{\Delta X, \Delta \lambda\} to estimate uncertainties

- method 1: pathways to dominant nuclides
- method 2: Monte-Carlo sensitivity
- method 3: reduced model Monte-Carlo sensitivity
• Pathways are used to identify the dominant contributors to the activation products for the specific irradiation scenario under consideration.

• This makes the calculation of uncertainties more practicable for all methods (random-walk approximation and Monte-Carlo).

• The standard uncertainty output uses a random-walk approximation to estimate error bounds.

• This estimate is much quicker than Monte-Carlo, but is likely to give larger bounds since it ignores many possible correlations.
• given initial inventory and irradiation scenario
• sort dominant nuclides at end of irradiation phase
  • \texttt{topxx} (=20) controls number
  • 8 categories - activity, heat production, dose, etc.

• construct pathways from initial to dominant nuclides
  • \texttt{path\_floor} (=0.005) and \texttt{loop\_floor} (=0.01)
  • iterate on single-visit breadth-first search tree

• compute inventory contributions of pathways
• construct error estimate
• keep pathways providing > path_floor of target inventory
• keep loop providing > loop_floor of pathway inventory
Error estimate

\[ Q = \sum_{t \in S_t} q_t; \quad (\Delta Q)^2 = \sum_{t \in S_t} \left( \frac{\Delta N_t}{N_t} \right)^2 q_t^2 \]

\[ (\Delta N_t)^2 = \sum_{p \in S_o} \Delta_{tp}^2 N_{tp}^2 + \sum_{a \in S_{sa}} \left( \sum_{p \in S_a} |\Delta_{tp}| N_{tp} \right)^2 \]

\[ \Delta_{tp}^2 = \sum_{e \in S_e} \sum_{r \in S_r} \left[ \frac{R_r \Delta_r}{R_e} \right]^2 + \sum_{e \in D_e} \left[ \frac{\Delta \lambda_e}{\lambda_e} \right]^2 \]

- \( N_t \) (atoms) and \( q_t \) (radiological quantity) from rate equation
- \( \Delta_{tp}, N_{tp}, \Delta N_t \) from pathways
- \( R_r \) and \( R_e \) pulse averaged reaction rates
- reactions uncorrelated, fission correlated
UNCERTAINTY ESTIMATES (cross sections only)
-------------------------------------------

Uncertainty estimates are based on pathway analysis for the irradiation phase
Total Activity is $1.25070 \times 10^{14} \pm 8.52 \times 10^{11}$ Bq. Error is $6.81 \times 10^{-1}$ % of the total.

Total Heat Production is $3.60059 \times 10^{-2} \pm 3.09 \times 10^{-4}$ kW. Error is $8.60 \times 10^{-1}$ % of the total.

Total Gamma Dose Rate is $5.63098 \times 10^{4} \pm 5.04 \times 10^{2}$ Sv/hr. Error is $8.95 \times 10^{-1}$ % of the total.

Total Ingestion Dose is $1.38528 \times 10^{5} \pm 1.17 \times 10^{3}$ Sv. Error is $8.45 \times 10^{-1}$ % of the total.

Target nuclide Sc 44 99.557% of inventory given by 8 paths
-------------------

path 1 20.048% Ti 46 ---(R)--- Sc 45 ---(R)--- Sc 44m---(b)--- Sc 44 ---(S)---
98.16%(n,np) 100.00%(n,2n) 1.84%(n,d)

path 2 12.567% Ti 46 ---(R)--- Sc 45 ---(R)--- Sc 44m---(b)--- Sc 44 ---(S)---
98.16%(n,np) 100.00%(n,2n) 100.00%(IT) 0.00%(n,n)

path 3 11.143% Ti 46 ---(R)--- Sc 45m---(d)--- Sc 45 ---(R)--- Sc 44 ---(S)---
96.62%(n,np) 100.00%(IT) 100.00%(n,2n) 3.38%(n,d)

...
• The TENDL library contains MF=33, LB=6 data for different reactions $X_1, X_2, \ldots$ for a given parent, i.e., $p(n, X_1)d_1, p(n, X_2)d_2, \ldots$.

• These covariance data $\text{cov}(X_1, X_2)$ for $X_1, X_2$ are stored as fractional values $f^{X_1X_2}$ and are tabulated in the same energy bins as used respectively for the LB=5 covariance data $f^{X_1X_1}, f^{X_2X_2}$ for reactions $X_1, X_2$.

• If the COVARIANCE keyword is used, FISPACT-II reads these data for all energy bins $k$ and $l$ and corrects for any instances where

$$\left| \frac{f^{X_1X_2}_{kl}}{\sqrt{f^{X_1X_1}_{kk} f^{X_2X_2}_{ll}}} \right| > 1$$
• Then the code uses the corrected data to compute collapsed covariance $\text{cov}(X_1, X_2)$. Covariances are mapped to MF=10 by assuming that all isomeric daughters of a given pair of reactions with rates $X_1$, $X_2$ have the same collapsed correlation function, $\text{corr}(X_1, X_2)$.

• Tables of all reactions which have covariance data and their collapsed covariances and correlations are printed by the collapse run. Inspection of these data will show those cases where the assumption of zero correlation between reactions of a given parent is not good.

• The effect of non-negligible correlations on uncertainties may be introduced into Monte-Carlo sensitivity calculations by choosing distributions of sample cross-sections to have the same variances and covariances as given by the TENDL data.
• reference run + S inventory calculations
• independent \{X_i^s; i = 1,\ldots, I; s = 1,\ldots, S\}
• dependent \{Y_j^s; j = 1,\ldots, J; s = 1,\ldots, S\}
• independent variables selected using random numbers
  ▪ normal, log-normal, uniform, log-uniform
  ▪ means \(\langle X_i \rangle\) and standard deviations \(\langle \Delta X_i \rangle\)
• compute summary results:
  ▪ means
  ▪ standard deviations
  ▪ Pearson correlation coefficients
• output full data for post-processing
• output mean and standard deviation

\[
\bar{X}_i = \frac{1}{S} \sum_{s=1}^{S} X_i^s \\
\Delta X_i = \sqrt{\frac{1}{S - 1} \sum_{s=1}^{S} [(X_i^s)^2 - \bar{X}_i^2]}
\]

\[
\bar{Y}_j = \frac{1}{S} \sum_{s=1}^{S} Y_j^s \\
\Delta Y_j = \sqrt{\frac{1}{S - 1} \sum_{s=1}^{S} [(Y_j^s)^2 - \bar{Y}_j^2]}
\]

• Pearson correlation coefficient

\[
\rho_{ij} = \frac{\sum_{s} X_i^s Y_j^s - S \bar{X}_i \bar{Y}_j}{\Delta X_i \Delta Y_j}
\]

• controlled by keywords SENSITIVITY, MCSAMPLE, MCSEED, COVARIANCE
Sample sensitivity output

Base cross section data

<table>
<thead>
<tr>
<th>index</th>
<th>i</th>
<th>zai</th>
<th>nuc_no</th>
<th>name</th>
<th>parent</th>
<th>daughter</th>
<th>sigma</th>
<th>sigma_unc</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<td>233</td>
<td>Ti 46</td>
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<td>219</td>
<td>Sc 46</td>
<td>0.39039E-25</td>
<td>0.35942E-01</td>
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<td>233</td>
<td>Ti 46</td>
<td>210461</td>
<td>220</td>
<td>Sc 46m</td>
<td>0.10142E-25</td>
<td>0.35942E-01</td>
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<tr>
<td>3</td>
<td>220480</td>
<td>235</td>
<td>Ti 48</td>
<td>210480</td>
<td>222</td>
<td>Sc 48</td>
<td>0.11049E-25</td>
<td>0.87272E-02</td>
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</table>

... Output nuclides

<table>
<thead>
<tr>
<th>j</th>
<th>i</th>
<th>zai</th>
<th>nuc_no</th>
<th>name</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>210460</td>
<td>219</td>
<td>Sc 46</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>210470</td>
<td>221</td>
<td>Sc 47</td>
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<td>3</td>
<td>210480</td>
<td>222</td>
<td>Sc 48</td>
<td></td>
</tr>
</tbody>
</table>

... Normal, x cutoff = [ -3.0000 , 3.0000 ] std dev ➜ Normal random sampling

<table>
<thead>
<tr>
<th>j</th>
<th>atoms_base</th>
<th>atoms_mean</th>
<th>atoms_unc</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.50290E+20</td>
<td>2.49955E+20</td>
<td>2.46164E-02</td>
</tr>
<tr>
<td>2</td>
<td>7.99801E+18</td>
<td>7.99665E+18</td>
<td>1.68690E-03</td>
</tr>
<tr>
<td>3</td>
<td>9.91006E+18</td>
<td>9.90588E+18</td>
<td>8.55649E-03</td>
</tr>
</tbody>
</table>

... Correlation coefficients ➜ reactions

<table>
<thead>
<tr>
<th>j \ i</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>9.66468E-01</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>-</td>
<td>-</td>
<td>1.00000E+00</td>
<td>-</td>
</tr>
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<td>-</td>
<td>9.99993E-01</td>
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<td>-</td>
<td>-</td>
<td>-</td>
</tr>
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<td>-</td>
<td>-</td>
<td>-9.60898E-01</td>
<td>-</td>
</tr>
<tr>
<td>7</td>
<td>-9.66478E-01</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

↑ output nuclides
• UKDD-2012 decay - 3873 nuclides
• calculation includes all nuclides in master index
• INDEXPATH generates reduced master index from pathways
  ▪ typically few 10s of nuclides
  ▪ number adjustable by pathway parameters
• reduced master index run vs full run to validate discards
• Monte-Carlo sensitivity for reduced master index runs
  ▪ faster + comparable answers
Self shielding of resonant channels

- Probability tables, sub-group method
- High fidelity resonances
Self shielding of resonant channels

CALENDF probability tables are used to model dilution effects in the computation of the effective cross-sections

\[
\sigma_{\text{eff}} (x, n) = \sigma_{\text{eff}} (g, x, n) \quad \text{and} \quad p (x, n) = p (g, x, n)
\]

where
- \( g \) = energy group number
- \( x \) = macro-partial (or total) index
- \( n \) = quadrature index

<table>
<thead>
<tr>
<th>cal-mt</th>
<th>description</th>
<th>mt in set</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>elastic scattering</td>
<td>2</td>
</tr>
<tr>
<td>101</td>
<td>absorption (no outgoing neutron)</td>
<td>102 103 107</td>
</tr>
<tr>
<td>18</td>
<td>fission total</td>
<td>18</td>
</tr>
<tr>
<td>4</td>
<td>inelastic scattering (emitting one neutron)</td>
<td>4 11</td>
</tr>
<tr>
<td>15</td>
<td>multiple neutron production (excluding fission)</td>
<td>5 16 17 37</td>
</tr>
</tbody>
</table>

Table 14: CALENDF mt number.
Fig. 1a Cross section versus energy

1b Exact PT distribution

1c PT discretisation

\[
\frac{1}{G} \int_{E_{\text{inf}}}^{E_{\text{sup}}} \sigma_t^n(E) dE = \int_{\sigma_{\text{min}}}^{\sigma_{\text{max}}} p(\sigma_t) \sigma_t^n d\sigma_t = \sum_{i=1}^{i=N} p_i \sigma_{t,i}^n
\]
The moments having been computed, the probability table is established:

\[
I(z) = \int \frac{p(x)}{1-zx} \, dx = \underbrace{M_0 + M_1 z + M_2 z^2 + \ldots + M_{2N-1} z^{2N-1}}_{2N \text{ moments}} + R_{2N} z^{2N}
\]

\[
= \underbrace{b_0 + b_1 z + b_2 z^2 + \ldots + b_{N-1} z^{N-1}}_{Q_{N,N-1} = \text{PADE approximant}} + R'_2 z^{2N}
\]

\[
= \frac{b_0 + b_1 z + \ldots + b_{N-1} z^{N-1}}{\prod_{i=1}^{N} (1-zx_i)} + R'_2 z^{2N} = \sum_i \frac{p_i}{1-zx_i} + R'_2 z^{2N}
\]

The second line is the Padé approximant that introduces an approximate description of higher moment order.
The effective cross section can be calculated from either the pointwise cross section or the probability table as follows:

\[
\sigma_{x,\text{eff,quad}}(\sigma_d) = \frac{\sum_{i=1}^{N} p_i \sigma_{x,i}}{\sum_{i=1}^{N} \frac{p_i \sigma_{x,i}}{\sigma_{t,i} + \sigma_{d}}} = \frac{\sum_{i=1}^{N} p_i}{\sum_{i=1}^{N} \frac{p_i}{\sigma_{t,i} + \sigma_{d}}}
\]

When the dilution is infinite this formula becomes:

\[
\sigma_{x,\text{eff,quad}} = \sum_{i=1}^{N} p_i \sigma_{x,i}
\]
Effective cross sections comparison

The probability tables from CALENDF are used in conjunction with fine 709 or 1102 group data. They are given at 3 temperatures: 293.6, 600 and 900 Kelvin.

From 0.1 eV to the end of the URR

Uniquely accessible SSF’s in the URR!!

Self Shielding Factor

The graph shows cross sections and ratios for different energy levels, comparing TENDL-2011 PREPRO and TENDL-2011 CALENDF.

40-Zr-90
The dilution $d(p; g)$ for a given nuclide $p$ and energy group $g$ is computed using a weighted sum over all the nuclides, $q = 1;Q$ in the mixture. The first approximation for the fraction $f_q$ uses the total cross-sections:

$$d^{(0)}(p, g) = \sum_{q=1, p\neq q}^{Q} f_q \sigma^{LIB-tot}(q, g) \frac{f_p}{f_p}$$

where

$$\sigma^{LIB-tot}(p, g) = \sum_{y=1}^{Y} \sigma^{LIB}(p, g, y)$$

Over the energy range for which the probability table data are available, the above approximation is iteratively refined using:

$$S^{(i)}(g) = \sum_{q=1}^{Q} f_q \sigma^{LIB-tot}(q, g) \left( \frac{\sigma^{tot}(q, g, d^{(i)}(q, g))}{\sigma^{tot}(q, g, \infty)} \right)$$

$$d^{(i+1)}(p, g) = \frac{S^{(i)}(g)}{f_p} - \sigma^{LIB-tot}(p, g) \left( \frac{\sigma^{tot}(p, g, d^{(i)}(p, g))}{\sigma^{tot}(p, g, \infty)} \right)$$
Effective cross section: dilution effects

Tungsten cross section @ 293.6K
Temperature effect

The effect is not negligible around the resonances.

Giant resonances dominate the reaction rate.

The effect is not negligible around the resonances.
Self shielding of resonant channels

- thin and thick target yields
- High fidelity resonance
• thin and thick target yields
• accounts approximately for target geometry
• applicable to thick targets
• handles foils, wires, spheres and finite cylinders
• uses one physical length scale to represent the target: the "effective length" y

<table>
<thead>
<tr>
<th>Type ID</th>
<th>Geometry</th>
<th>Dimension(s)</th>
<th>Y</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>foil</td>
<td>thickness (t)</td>
<td>y=1.5t</td>
</tr>
<tr>
<td>2</td>
<td>wire</td>
<td>radius (r)</td>
<td>y=2r</td>
</tr>
<tr>
<td>3</td>
<td>sphere</td>
<td>radius (r)</td>
<td>y=r</td>
</tr>
<tr>
<td>4</td>
<td>cylinder</td>
<td>radius (r), height (h)</td>
<td>y=1.65rh(r+h)</td>
</tr>
</tbody>
</table>
• theory of radioisotope production
• production rates and cross-sections
• saturation factors and practical yields

• model uses resonance parameters from the Resolved Resonance Range
• model includes the effects of neutron loss through radiative capture
• model includes effects of neutron energy diffusion through elastic scattering
• one resonance in a pure target
• dimensionless parameter to combine the physical effective length with the nuclear parameters

\[ z = \sum_{\text{tot}} (E_{\text{res}}) \cdot y \sqrt{\frac{\Gamma_{\gamma}}{\Gamma}} \]

• where
  - \( \sum_{\text{tot}} (E_{\text{res}}) \) is the macroscopic cross-section at the energy \( E_{\text{res}} \) of the resonance peak
  - \( \Gamma_{\gamma} \) is the radiative capture width
  - \( \Gamma \) is the total resonance width
  - \( y \) “effective length”
• Self-shielding factor \( G_{\text{res}} \) is defined in terms of \( z \) only
Baumann, 1963; Yamamoto and Yamamoto, 1965; Lopes, 1991

$z = \Sigma_{\text{tot}}(E_{\text{res}}) \cdot y \cdot (\frac{\Gamma_{\gamma}}{\Gamma})^{1/2}$

Target geometry

Experimental self shielding factor

$z = \Sigma_{\text{tot}}(E_{\text{res}}) \cdot y \cdot (\frac{\Gamma_{\gamma}}{\Gamma})^{1/2}$
Model development, first step (2)

\[ G_{res}(z) = \frac{A_1 - A_2}{1 + \left( \frac{z}{\bar{z}_0} \right)^p} + A_2 \]

- this is the “universal sigmoid curve” for the model
- the parameters have been determined empirically to be a good fit to experimental data
- preferred values are:
  - \( A_1 = 1.000 \pm 0.005 \)
  - \( A_2 = 0.060 \pm 0.011 \)
  - \( \bar{z}_0 = 2.70 \pm 0.09 \)
  - \( p = 0.82 \pm 0.02 \)
• extend model to a group of separated resonances
• still considering a pure target: one nuclide
• assign a weight to each resonance

\[ w_i = \left( \frac{\Gamma_y}{E_{res}^2} \cdot \frac{g \Gamma_n}{\Gamma} \right)_i \]

where

- \( \Gamma_n \) is the neutron scattering width
- \( g \) is the statistical factor, \((2J + 1)/(2(2I + 1))\)
- \( J \) is the spin of the resonance state
- \( I \) is the spin of the target nucleus
- form an average self-shielding factor from all resonances of interest

\[ \langle G_{res} \rangle = \frac{\sum w_i G_{res}(z_i)}{\sum w_i} \]
• extend $\langle G_{\text{res}} \rangle$ to form the average for resonances of a mixture of nuclides
• assume the resonances of different nuclides do not overlap significantly
• make $\langle G_{\text{res}} \rangle$ energy dependent by taking averages separately for each energy bin used for the group-wise cross-sections
• use Fröhner’s simple expression for the peak cross-section of each resonance (not available from the GENDF data)
universal curve model provides an alternative to probability table self shielding

use $\langle G_{\text{res}} \rangle(E)$ to scale down energy-dependent cross-sections before cross-section collapse

$\langle G_{\text{res}} \rangle(E)$ reduces the neutron flux, so apply it to all cross-sections

target geometry specified with

$$\text{SSFGEOMETRY} \text{ type } \text{length}_1 \text{ <length}_2 \text{ >}$$

use resonances from mixture specified with $\text{SSFFUEL}$ or $\text{SSFMASS}$

PRINTLIB 6 now generates a table of all cross-sections with $\langle G_{\text{res}} \rangle$ reduction factors
Neutron-irradiated tungsten: comparison between experiment and simulation
• W irradiated in the high-flux reactor (HFR) @ NRG, Petten
• Has been cooling for a number of years (see later)
• Only now is it starting to be analyzed
• Full of defects & voids, and some percentage of transmutation products – mostly rhenium

Energy-dispersive X-ray spectroscopy:

- EDS spectral analysis: 8.6 keV corresponds to X-ray emission from Re
- Allows (surface) Re content to be quantified with good accuracy

Petten Single Crystal (1.2wt% Re measured)

Petten Polycrystalline (1.4wt% Re measured)
• W irradiated under EXTREMAT-II in 2008 & 2009
• Target of 282 days of irradiation (10 cycles), but in fact only irradiated in 8 cycles & in two different positions:

<table>
<thead>
<tr>
<th>Position</th>
<th>Cycle</th>
<th>EFPD</th>
<th>Start date</th>
<th>End date</th>
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<td>22-May-08</td>
<td>22-Jun-08</td>
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<tr>
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<td></td>
<td>09-May</td>
<td>17.61</td>
<td>30-Jun-09</td>
<td>18-Jul-09</td>
</tr>
<tr>
<td></td>
<td>09-Jun</td>
<td>22.06</td>
<td>17-Aug-09</td>
<td>08-Sep-09</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>208.26</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

• EFPD – effective full power days
• Samples were positioned next to another experiment with very strong thermal neutron absorption properties
  – W exposed to a lower than normal (for HFR) fraction of thermal neutrons creating reduced transmutation

• New spectra calculated for the approximate axial position of EXTREMAT-II, averaged over radial extent of experiment and over around 4 cm of height

Total fluxes for three spectra: 5.3 x 10^{14}, 6.61 x 10^{14}, 6.83 x 10^{14} n cm^{-2} s^{-1}, for original, C7, and C3, respectively
• To correctly account for self-shielding in all isotopes of W
  ▪ During collapse:

    PROBTABLE 1 1
    SSFCHOOSE 1 0 W
    SSFMASS 1.0 1
    W 100.0
    GETXS 1 709

• Other option (SSFUEL) allows explicit specifications of isotopes to self-shield
Important Reactions

• Main Re isotopes produced during irradiation are $^{185}\text{Re}$ and $^{187}\text{Re}$
  
  – Produced via $(n,\gamma)$ reactions on $^{184}\text{W}$ and $^{186}\text{W}$, followed by $\beta$-decay of $^{185}\text{W}$ ($T_{1/2} = 75$ days) and $^{187}\text{W}$ (24 hours), respectively.

• Raw total collapsed reaction rate (RR) for these $(n,\gamma)$ reactions and self-shielding (SS) corrected values:

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Original spectrum</th>
<th>C7</th>
<th>C3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Raw RR</td>
<td>SS RR</td>
<td>Raw RR</td>
</tr>
<tr>
<td>$^{186}\text{W}(n,\gamma)^{187}\text{W}$</td>
<td>22.5 (0.01)</td>
<td>17.2</td>
<td>6.21 (0.09)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(-72%)</td>
</tr>
<tr>
<td>$^{184}\text{W}(n,\gamma)^{185}\text{W}$</td>
<td>0.92 (0.71)</td>
<td>0.60</td>
<td>0.63 (1.8)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(-32%)</td>
</tr>
</tbody>
</table>

(all RR in barns, black bracket values are +/- errors, green bracket values are % reduction in RR relative to original spectrum)
• Almost 50% of RR comes from thermal neutrons below 10 eV

\[ ^{186}W(n,\gamma)^{187}W \]
For new spectra, only 20% of RR comes from thermal neutrons below 100 eV.

$^{184}\text{W}(n,\gamma)^{185}\text{W}$

(RR and $\sigma$ in a fine group structure with 660 bins below 30 MeV)
• Inventory simulation with FISPACT-II of pure tungsten with fully detailed irradiation schedule (including gaps and change in position) and new spectra
  – TENDL 2014 nuclear libraries in 660 energy groups
  – Self-shielding correction of reaction cross sections included (2% Re predicted without correction)

• Results after 208.26 effective full power days:
  – 1.4 atomic % Re (and 0.1% Os)
    • good agreement with 1.2-1.4% values from measurements
    • And much better than ~4% prediction based on usual HFR neutron spectrum
  – 1.6 effective dpa in the tungsten (using $E_d = 55$ eV)
A proper characterization of the neutron spectra for irradiated samples is vital to get even close to real transmutation rate in simulations

- Without this correct treatment of the neutron fields the reaction rates (and hence transmutation rates) for key capture reactions are much greater
- The thermal part of the neutron spectrum is very important and must be correctly predicted

Simulations in W with more realistic neutron spectra give Re production rates that are in very good agreement with experimental measurements

Further explorations:
- Properly corrected neutron spectra for W at the sample positions may cause further refinement of results
- Variation (of Re %) with depth due to self-shielding
• Collaboration with PSI, using modern CASMO-SIMULATE to compare inventory predictions for variety of assemblies:
  - BWR and PWR with mix of UO2, MOX, Gd
  - Includes Takahama, Atrium-10, TMI-1, Beznau
• Added 586 CASMO data for ENDF/B-VII.1, with CALENDF PTs for self-shielding. Applied to major actinides, but can in principle apply to any nuclide
• **Left**: U8 capture RR and SSFs  **Right**: U5 fission RR+SSFs

Note: CASMO 586 treatment of <10 eV requires no SSFs! No so for >10 eV, where significant SS occurs and must be accounted for.
• In all examples, normalisation using POWER keyword of FISPACT-II (normalising flux based on full Kerma) to CASMO power density, converted to W/cc.

• Ratios are to CASMO simulation, following the spectra changes over 40 GWd/te, below: BWR MOX simulation