Reaction rate uncertainty quantification and propagation

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Boltzmann equation
transport
time independent
energy and spatial simulation
primary response

Bateman equation
inventory
time dependent
secondary response

VESTA, MCR2S, ...
... interfaces to connect Boltzmann and Bateman solvers for non-linear t- and T-dependent transport
EASY-II framework

- FISPACT-II is a modern engineering prediction tool for activation-transmutation, depletion inventories at the heart of the EASY-II system that relies on the n-TAL collaboration to provide the nuclear data libraries.
- FISPACT-II was designed to be a functional replacement for the code FISPACT-2007 but now includes enhanced capabilities.
- $\alpha$, $\gamma$, d, p, n-Transport Activation Library: TENDL-2012 from the TENDL collaboration, but also ENDF/B, JENDL, JEFF
- All nuclear data processing is handled by NJOY (LANL), PREPRO (LLNL), and CALENDF (CEA-CCFE)
- Set of stiff differential equations to be solved

\[
\frac{dN_i}{dt} = -N_i (\lambda_i + \sigma_i \varphi) + \sum_{j \neq i} N_j (\lambda_{ij} + \sigma_{ij} \varphi)
\]

- Here \( \lambda_i \) and \( \sigma_i \) are respectively the total decay constant and cross-section for reactions on nuclide I.

- \( \sigma_{ij} \) is the cross-section for reactions on nuclide j producing nuclide i, and for fission it is given by the product of the fission cross-section and the fission yield fractions, as for radionuclide production yield.

- \( \lambda_{ij} \) is the constant for the decay of nuclide j to nuclide i.
Rate equations: numerical aspects

- **LSODES**, Livermore Solver for Ordinary Differential Equations solves stiff (stiff ode are evil) and non stiff systems, efficient handling of sparse Jacobian matrices
  - Backward Differentiation Formula (BDF) methods (Gear’s method) in stiff cases to advance the inventory
  - Adams methods (predictor-corrector) in non stiff case
  - Yale sparse matrix for linear systems
  - ability to handle time-dependent matrix
  - no need for equilibrium approximation
  - handles short (1ns) time interval and high fluxes
- LSODES wrapped in portable Fortran 95 code
  - dynamic memory allocation
  - minor changes to Livermore code to ensure portability
EASY-II TENDL’s libraries – 1 GeV

- n-tendl-2012 (2011), multi temperature, 709 group library; 2434 targets
  - full set of covariance
  - probability tables in the RRR and URR

- γ-tendl-2012, 162 group library, 2430 targets
- p-tendl-2012, 162 group library, 2429 targets
- d-tendl-2012, 162 group library, 2428 targets
- α-tendl-2012, 162 group library, 2429 targets

- EAF-2007 libraries; 293K, 816 targets (55 MeV)
- EAF-2010 libraries; 293K, 816 targets (55 MeV)
- EAF uncertainty file
EASY-II other libraries

- Decay-2012, 3873 isotopes (23 decay modes; 7 single and 16 multi-particle ones)
- Ingestion and inhalation, clearance and transport indices libraries, 3873 isotopes
- JEFF-3.1, UKFY4.1 fission yields

- EAF-2010 decay data: 2233 isotopes
- EAF-2010 ingestion and inhalation, clearance and transport indices libraries, 2233 isotopes
Processing steps: burnup, transmutation

• Multi-particles groupwise, multi-temperature libraries with NJOY-99.393, PREPRO-2012, probability tables in the RRR & URR with CALENDF-2010
  
  ▪ For the inventory code FISPACT-II

• From $\alpha, \gamma, p, d, n$-TENDL-2012 (2011)

• FISPACT-II parses directly the TENDL’s covariance information

• Transport and activation application libraries now stem from unique, truly general purpose files
FISPACT-II irradiation scenarios

- 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
What FISPACT-II does

- 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
Extract and reduce library data

- 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
  - Data used in code
    - collapsed cross-section $\overline{XS}$
    - collapsed uncertainty $\Delta$

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

\[ \overline{XS} = \sum_{i=1}^{n} W_i X_i \]
• 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 $\overline{XS}$

$$\text{var} = \sum_{i=1}^{N} \sum_{j=1}^{N} W_i W_j \text{Cov}(X_i, X_j); \quad 1 \text{ TENDL, 3 EAF} \quad \Delta = \{1|3\} \sqrt{\text{var}} / \overline{X}$$

• 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 $S^k_i$ maps cross-section energy bins to covariance energy bins:

$$S^k_i = \begin{cases} 
1 & \text{bin } i \text{ in bin } k \\
0 & \text{otherwise} 
\end{cases}$$

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

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

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

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

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

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

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
  • topxx (=20) controls number
  • 8 categories - activity, heat production, dose, etc.
• construct pathways from initial to dominant nuclides
  • path_floor (=0.005) and 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 6.81E-01 % of the total.

Total Heat Production is \(3.60059 \times 10^{-2} \pm 3.09 \times 10^{-4}\) kW. Error is 8.60E-01 % of the total.

Total Gamma Dose Rate is \(5.63098 \times 10^{4} \pm 5.04 \times 10^{2}\) Sv/hr. Error is 8.95E-01 % of the total.

Total Ingestion Dose is \(1.38528 \times 10^{5} \pm 1.17 \times 10^{3}\) Sv. Error is 8.45E-01 % 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 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)
       1.84%(n,d) 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 $X_1, X_2, ...$ for a given parent, i.e., $p(n, X_1)d_1$, $p(n, X_2)d_2$, ... .

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

$$\left| \frac{f^{X_1X_2}}{\sqrt{f^{X_1X_1}f^{X_1X_1}}} \right| > 1$$
Using LB = 6 data

• 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.
Uncertainty from sensitivity calculation

- reference run + S inventory calculations
- independent \( \{X^s_i \; ; i = 1,\ldots,l; s = 1,\ldots,S\} \)
- dependent \( \{Y^s_j \; ; j = 1,\ldots,J; s = 1,\ldots,S\} \)
- 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
Monte Carlo approach to sensitivity analysis

- output mean and standard deviation

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

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

- Pearson correlation coefficient

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

- controlled by keyword SENSITIVITY, MCSAMPLE, MCSEED, COVARIANCE
### Sample sensitivity output

#### Base cross section data

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#### Output nuclides

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#### Normal, x cutoff = [ -3.0000 , 3.0000 ] std dev  

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...  

#### Correlation coefficients

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↑ output nuclides

↔ Normal random sampling
Uncertainty from reduced models

- EAF-2010 - 2233 nuclides,
- TENDL-2012 - 3873 nuclides
- calculation includes all nuclides in master index
- INDEXPATH generates reduced master index from pathways
- reduced master index run vs full run to validate discards
- Monte-Carlo sensitivity for reduced master index runs
Verification and Validation V&V

• Differential
  ▪ C/E with the latest EXFOR, C/C with EAF’s, ENDF’s files
  ▪ SACS: Statistical Analysis of Cross Section; Kopecky & Forrest legacy systematics.

• Integral
  ▪ Criticality
    • TRIPOLI-4.9 ICSBEP suite (130 cases)
    • MCNP6 ‘SvdM NRG’ ICSBEP suite (1900 cases)
  ▪ Transport, shielding
    • MCNP6 ‘SvdM NRG’ Sinbad and LLNL suites

➤ Activation-transmutation; activity, gamma, decay heat
  • EASY-II validation suite (500 reaction rates, thousands of integral E, time dependent, fusion orientated)

• MACS and RI: Maxwellian-averaged cross sections and astrophysical reaction rates, resonance integrals
14 MeV neutrons are generated by a 2 mA deuteron beam impinging on a stationary tritium bearing titanium target; Fusion Neutron Source (FNS) Neutron spectra, neutron fluence monitored by $^{27}\text{Al}(n,\alpha)^{24}\text{Na}$

Two experimental campaigns: 1996 and 2000; 74 materials

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<td>Hg</td>
<td>HgO</td>
</tr>
<tr>
<td>42</td>
<td>Mo</td>
<td>Metallic Foil</td>
<td>81</td>
<td>Ti</td>
<td>TiO</td>
</tr>
<tr>
<td>44</td>
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<td>Pb</td>
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</tr>
<tr>
<td>45</td>
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<td>83</td>
<td>Bi</td>
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<tr>
<td>46</td>
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<td>87</td>
<td>Ni</td>
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</tr>
<tr>
<td>47</td>
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<td>88</td>
<td>Cr</td>
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<td>48</td>
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<td>89</td>
<td>Si</td>
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<td>49</td>
<td>In</td>
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<td>90</td>
<td>Mo</td>
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</table>

FNS Neutron spectra, neutron fluence monitored by $^{27}\text{Al}(n,\alpha)^{24}\text{Na}$
Decay power: FNS JAERI Cr

FNS-00 5 Min. Irradiation - Cr

<table>
<thead>
<tr>
<th>Product</th>
<th>Pathways</th>
<th>$T_{1/2}$</th>
<th>Path %</th>
<th>E/C</th>
</tr>
</thead>
<tbody>
<tr>
<td>V52</td>
<td>Cr52(n,p)V52</td>
<td>3.7m</td>
<td>98.1</td>
<td>0.99</td>
</tr>
<tr>
<td></td>
<td>Cr53(n,d+np)V52</td>
<td>-</td>
<td>1.9</td>
<td>0.99</td>
</tr>
<tr>
<td>Cr49</td>
<td>Cr50(n,2n)Cr49</td>
<td>41.9m</td>
<td>100.0</td>
<td>1.82</td>
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</tbody>
</table>

Heat Output [µW/kg] vs. Time after irradiation [minutes]

Products: V52, V53, Cr50, Ti51, Cr49
### Decay Power: FNS JAERI Cr

#### Impurities could have been present in the sample at levels up to 2000 and 6000 ppm, as it has been measured in the same type of sample.

<table>
<thead>
<tr>
<th>Times</th>
<th>FNS EXP. 5 mins</th>
<th>TENDL-2012</th>
<th>E/C</th>
<th>TENDL-2011</th>
<th>E/C</th>
<th>EAF-2010</th>
<th>E/C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min.</td>
<td>µW/g</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>0.58</td>
<td>1.68E+00</td>
<td>1.76E+00</td>
<td>0.96</td>
<td>1.76E+00</td>
<td>0.95</td>
<td>1.76E+00</td>
<td>0.95</td>
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<td>1.66E+00</td>
<td>0.95</td>
<td>1.66E+00</td>
<td>0.95</td>
<td>1.67E+00</td>
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<tr>
<td>1.10</td>
<td>1.51E+00</td>
<td>1.58E+00</td>
<td>0.96</td>
<td>1.58E+00</td>
<td>0.95</td>
<td>1.58E+00</td>
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<tr>
<td>1.37</td>
<td>1.44E+00</td>
<td>1.49E+00</td>
<td>0.96</td>
<td>1.49E+00</td>
<td>0.96</td>
<td>1.50E+00</td>
<td>0.96</td>
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<tr>
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<td>1.37E+00</td>
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<td>1.42E+00</td>
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<td>1.30E+00</td>
<td>0.97</td>
<td>1.30E+00</td>
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<td>0.98</td>
<td>1.16E+00</td>
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</tr>
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<td>0.98</td>
<td>1.02E+00</td>
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<tr>
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<tr>
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<td>5.66E-01</td>
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<td>19.33</td>
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<td>5.06E-02</td>
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<td>1.33E-03</td>
<td>1.66</td>
<td>1.11E-03</td>
<td>2.00</td>
</tr>
</tbody>
</table>

#### Product Pathways

- **V52**
  - Cr52(n,p)V52
  - Cr53(n,d+np)V52
- **Cr49**
  - Cr50(n,2n)Cr49

<table>
<thead>
<tr>
<th>Product</th>
<th>Pathways</th>
<th>T₁/₂</th>
<th>Path %</th>
<th>E/C</th>
<th>ΔE%</th>
</tr>
</thead>
<tbody>
<tr>
<td>V52</td>
<td>Cr52(n,p)V52</td>
<td>3.7m</td>
<td>98.1</td>
<td>0.99</td>
<td>7%</td>
</tr>
<tr>
<td></td>
<td>Cr53(n,d+np)V52</td>
<td></td>
<td>1.9</td>
<td>0.99</td>
<td>7%</td>
</tr>
<tr>
<td>Cr49</td>
<td>Cr50(n,2n)Cr49</td>
<td>41.9m</td>
<td>100.0</td>
<td>1.82</td>
<td>6%</td>
</tr>
</tbody>
</table>
Decay power: FNS JAERI Inconel 600

random-walk

FNS-00 5 Min. Irradiation - Inc600

<table>
<thead>
<tr>
<th>Product</th>
<th>Pathways</th>
<th>$T_{1/2}$</th>
<th>Path %</th>
<th>E/C</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{52}$V</td>
<td>$^{52}$Cr (n, p) $^{52}$V</td>
<td>3.7m</td>
<td>95.9</td>
<td>1.20</td>
</tr>
<tr>
<td></td>
<td>$^{53}$Cr (n, d) $^{52}$V</td>
<td>1.2</td>
<td>1.20</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$^{55}$Mn (n, a) $^{52}$V</td>
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<td>1.20</td>
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<td>2.5h</td>
<td>99.5</td>
<td>1.03</td>
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</table>

Heat Output [µW/kg] vs Time after irradiation [minutes]
FNS-00 5 Min. Irradiation - Y$_2$O$_3$

<table>
<thead>
<tr>
<th>Product</th>
<th>Pathways</th>
<th>$T_\frac{1}{2}$</th>
<th>Path %</th>
<th>E/C</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{16}$N</td>
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<td>7.1s</td>
<td>99.9</td>
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<tr>
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<td>$^{89}$Y (n, n') $^{89m}$Y</td>
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<td>1.03</td>
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<tr>
<td>$^{86m}$Rb</td>
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<tr>
<td>$^{88}$Y</td>
<td>$^{89}$Y (n, 2n) $^{88}$Y</td>
<td>106.6d</td>
<td>100.0</td>
<td>0.99</td>
</tr>
</tbody>
</table>

Heat Output [µW/kg] vs Time after irradiation [minutes]

FNS Experiment —
EAF-2010 ———
TENDL-2011 ———
TENDL-2012 ————

Random-walk

Y

Rb

N

O (n, p)

89mY

86mRb

88Y

89mY

86mRb

88Y

89mY

86mRb

88Y

89mY

86mRb

88Y

89mY

86mRb

88Y

89mY

86mRb

88Y
FISPACT-II:

- A powerful activation-transmutation prediction tool
- Identifies and quantifies important reactions and decays
- Uses full TENDL-2012 covariance data
- Uncertainty estimates:
  - pathways to dominant nuclides
  - Monte-Carlo sensitivity
  - reduced model + Monte-Carlo sensitivity
- Uncertainty on all responses: activity, decay heat, dose rate, inhalation and ingestion indices, ….

http://www.ccfe.ac.uk/EASY.aspx