Use of Fission Data in MCNP6
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Outline

- Introduction
- Detection - Fission multiplicity
- Detection - Delayed particles
- Burnup – Fission yields, Q value
- Summary
Neutron Signatures

Spontaneous fission

Pu-240 → Zr-103 → Xe-134

Number of neutrons emitted

Probability

(alpha, n) neutrons

O-17 → Ne-20

single neutron only

Induced fission

Pu-239 + Mo-105 → Xe-134 + Te-133

Pu-240 Xe-134

Zr-103

Ne-20

O-17

single neutron only

Pu-239

Te-133

Mo-105
Passive Neutron Counter

- **3He neutron detectors**
- **Fissioning source surrounded by neutron detectors**
- **Prompt multiple neutron emission from fission detected as coincidence neutron events**
- **Pulse processing electronics count the S and D count rates, which are used to calculate the mass of fissioning isotopes**
HLNCC

- JUNCTION BOX
- SHIELD PLANE
- ELECTRONICS
- 3He TUBES (18)
- POLYETHYLENE
- ALUMINIUM
- Cd LINERS

Measurements:
- 34.0
- 17.5
- 41.0
- 12.6
- 8.3
- 68.2
Multiplicity Treatments in MCNP

Several options for simulating fission multiplicity have been added to MCNP in the last few years.

- Spontaneous multiplicities from Enslinn (LA-13422)
- Induced multiplicities from Lestone (LA-UR-05-0288)
- LLNL Fission Library (UCRL-AR-228518)

Invoked with FMULT card

- “All or nothing” approach - the chosen multiplicity model is applied to all fissions (SF and Induced).
Fission Multiplicity Treatments in MCNP

- Start a thermal neutron in U-235
- 83.7% Fissions
- All results use the Tally Probability Density Function to compare history scores (modified to score in integer values).
- Run neutron source in sphere with 1\textsuperscript{st} interaction (lca 7j -2).
- Tally crossings (F1) and energy of crossings (*F11) on sphere surface.
- Neutron multiplicities should agree overall for most physics.
- Total Neutron Energy per Fission should show higher “tail” for uncorrelated treatments. Large multiplicity values sample from same energy functions resulting in higher energy totals.
- Compare Integer sampling, default multiplicity treatment (Lestone), LLNL library and FREYA.
Neutron Multiplicity

Mean Values
Int. Samp 2.06
Lestone 2.06
LLNL 2.06
FREYA 2.06
Total Neutron Energy per fission

Mean values
Int. samp 4.12
Lestone 4.12
LNLL 3.90
FREYA 3.89
Angular Correlation

- Place source in cube, run 1st interaction (lca 7j -2).
- Tally on opposite faces and adjacent faces.
  - 3 tallies on opposite facets (1.1+1.2, 1.3+1.4, 1.5+1.6)
  - 3 tallies on adjacent facets (1.1+1.5, 1.2+1.4, 1.3+1.6)
- If neutron emissions correlate along vector line, then opposite faces should see higher neutron counts/multiplicities.
LLNL Fission Library

LLNL is isotropic and uncorrelated, all tallies are identical.
FREYA results show three opposite-surface tallies are larger than three adjacent-surface (curves are displayed with small x-axis offsets for clarity).
Fission Neutron Multiplicity

- Standards MCNP6 Treatment is integer sampling.
- Several fission models can be used for multiplicity.
- All emit uncorrelated neutrons in energy and angle.
- Mode detailed physics (CGMF and/or FREYA) would provide better detailed distributions with correlations.
Fission Gamma Multiplicity

- Standard Treatment in MCNP6 is integer sampling.
- LLNL Fission library provides Gaussian distribution.
- Need better model for correlations to preserve spectra/energy and multiplicity?
Fission Gamma Multiplicity

Base fission gamma multiplicity in MCNP6 (blue) compared to LLNL fission model (black).
Fission Gamma Multiplicity

Fission gamma spectrum in MCNP6 (blue) compared to LLNL fission model (black).
Fission Gamma Multiplicity

Overall Fission gamma energy in MCNP6 (blue) compared to LLNL fission model (black).

Gamma energy/fission:
Default: 6.44
LLNL:  5.83
Delayed Particle Physics

- The need arose to compute signals from active interrogation scenarios.
- Leverage the existing CINDER code in MCNP to produce time-dependent isotopics.
- Fission sampling uses existing fission product distributions in CINDER (cinder.dat).
- FP Distributions are from
  - Thermal reactor
  - Fast Reactor
  - 14-MeV source
- MCNP can integrate over FP distribution to gather either coarse binwise spectrum of 25 groups or detailed line spectrum.
CINDER90 in MCNP6

- What is there?
  - FP yields for many isotopes at 3 energies
  - Decay information for 3360 isotopes (half-life, branching ratios, decay products)
  - 25 group decay gamma spectra
  - 63 group cross sections for many reactions.
  - Mostly from ENDF/B-VI
  - Photonuclear FP yields from GEF* Code added by NEN-5.

CINDER90 in MCNP6 – cont.

- What is there?
  - Markov chain solver for evolution of isotopes.
  - Post-processing code reports decay gamma spectra at each time step.
Qualitative benchmark of DG

- Compared results to Beddingfield experiments.
- Much of the structure was captured although some differences were also clear.
Delayed Neutrons

- MCNP has historically done delayed particles using six-group formulation from ENDF and sampling a specified energy spectrum.
- The delayed particle feature allows us to build a custom delayed-neutron precursor from the FP set and sample for time and energy.
- Data files delay_library_v3.dat contains decay neutron information for 279 isotopes.
- This process is much slower!
DN from U-235 Results

DN Fraction:
ENDF: 0.00656
MCNP/CINDER 0.00773
DN from Pu-239 Results

DN Fraction:
ENDF: 0.00226
MCNP/CINDER 0.00257
DN Spectra

U-235 ENDF
U-235 MCNP/CINDER
Pu-239 ENDF
Pu-239 MCNP/CINDER
Burnup/Depletion Capability in MCNP6

- Show flowchart
- Ability to track isotopic evolution in critical systems.
- Relies on CINDER for data/algorithms.
Monte Carlo Linked Depletion Process

- Steady state Monte Carlo using MCNPX, depletion utilizing CINDER90
Predictor Corrector

\[ N(r,t) = N(r,0)e^{-\sum_{i=0}^{E} \int_{t_0}^{t_1} \sigma(r,E)\phi(r,t')dt'} \]

- \( \sum \sigma(r,E) \int \phi(r,t')dt' \)

Number Density

FLUX

- Monte Carlo: Time = \( t(i) \) Initial collision densities/fluxes Initial number densities \( (N_0) \)
- CINDER90: Depletion Calculation \([t(i) \rightarrow t(i+1/2)]\) Calculate New Number Densities
- Monte Carlo: Time = \( t(i+1/2) \) Recalculate collision densities/fluxes
- CINDER90: Rerun Depletion Calculation \([t(i) \rightarrow t(i+1)]\) Use recalculated collision densities/fluxes Calculate New Number Densities = \( N_c \)
- For next sequence of time steps \( N_0 = N_c \)

Final Time Step

No

Yes

Done
FP Yield Energy Dependence
FP Yield Data Available

- Transmutation chain data for 3400 isotopes
- Fission Yield Data for 1325 isotopes
FP Yield Nuclide Dependence

Open Cinder.dat
- Go to second “#3215"
- 12,13,14 =(n,f) yield sets
- Go to “Fission Yield”
Recoverable Energy per Fission

\[ Q_{\text{recoverable}} = Q_{\text{prompt}} + Q_{\text{delayed}} + (\bar{v}(E) - k_{\text{eff}}) * Q_{\text{capture}} \gamma - Q_{\text{neutrino}} \]

- **Prompt Q value** is usually determined from ENDF tape
  - File 1 MT 458

- **Delayed Q value** may be estimated assuming local energy deposition
  - Deposited gamma energy may need adjustment
    - 207 of 390 isotopes contain capture gamma data in ENDF VII.0

- **Prompt Q not available** for all actinides.
  - Qfis array on MCNP is incomplete and ad-hoc (ENDF-VI, JEFF-3.1, ??)
  - Data present for 22 isotopes (64 actinides in ENDF-VII)
  - Capture gamma data incomplete.

### Emitted and recoverable energy for fission of U-235

<table>
<thead>
<tr>
<th>Form</th>
<th>Emitted Energy (MeV)</th>
<th>Recoverable Energy (Mev)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fission Fragments</td>
<td>168</td>
<td>168</td>
</tr>
</tbody>
</table>
| Fission Product Decay
  - \( \gamma \)-rays          | 8                    | 8                        |
  - \( \beta \)-rays           | 7                    | 7                        |
| neutrinos                     | 12                   | --                       |
| Prompt gamma rays             | 7                    | --                       |
| Fission neutrons (kinetic energy) | 5                 | 5                        |
| Capture \( \gamma \)-rays    | --                   | 3-12                     |
| **Total**                     | **207**              | **198-207**              |
H. B. Robinson

- 15 X 15 Westinghouse fuel assembly from H. B. Robinson Unit 2
  - ORNL/TM-12667
  - ENDF/B VII.0 temperature dependent library
  - 16.02, 23.8, 28.47, and 31.66 GWD/MTU

<table>
<thead>
<tr>
<th>Cycle</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
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<tbody>
<tr>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Operating Interval (days)</td>
<td>243.5</td>
<td>243.5</td>
<td>156</td>
<td>156</td>
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<tr>
<td>Downtime (days)</td>
<td>40</td>
<td>64</td>
<td>39</td>
<td>--**</td>
</tr>
<tr>
<td>Average Soluble Boron Concentration (ppm)</td>
<td>625.5</td>
<td>247.5</td>
<td>652.5</td>
<td>247.5</td>
</tr>
</tbody>
</table>

** 3936 for Cases A-B or 3637 for Cases C-D
## Results

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Case A 16.02 GWD/MTU</th>
<th>Case B 23.8 GWD/MTU</th>
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<tbody>
<tr>
<td></td>
<td>MCNP6</td>
<td>MCNPX</td>
</tr>
<tr>
<td>235U</td>
<td>3.73</td>
<td>0.42</td>
</tr>
<tr>
<td>236U</td>
<td>-3.43</td>
<td>-1.76</td>
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<tr>
<td>238U</td>
<td>0.06</td>
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<tr>
<td>238Pu</td>
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<tr>
<td>239Pu</td>
<td>5.59</td>
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<tr>
<td>240Pu</td>
<td>2.66</td>
<td>3.32</td>
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<tr>
<td>241Pu</td>
<td>7.68</td>
<td>3.57</td>
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<tr>
<td>237Np</td>
<td>-3.23</td>
<td>-6.13</td>
</tr>
<tr>
<td>99Tc</td>
<td>8.49</td>
<td>10.91</td>
</tr>
<tr>
<td>137Cs</td>
<td>-3.06</td>
<td>-1.12</td>
</tr>
</tbody>
</table>
## Results

### Case C

<table>
<thead>
<tr>
<th>Isotope</th>
<th>MCNP6</th>
<th>MCNPx</th>
<th>SCALE</th>
<th>MONTEBURNS</th>
</tr>
</thead>
<tbody>
<tr>
<td>235U</td>
<td>-3.27</td>
<td>-11.80</td>
<td>-4.90</td>
<td>-2.44</td>
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<tr>
<td>236U</td>
<td>1.84</td>
<td>3.72</td>
<td>2.20</td>
<td>1.24</td>
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<tr>
<td>238U</td>
<td>0.47</td>
<td>0.47</td>
<td>0.50</td>
<td>0.54</td>
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<tr>
<td>238Pu</td>
<td>-11.04</td>
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<td>-1.77</td>
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<td>240Pu</td>
<td>2.09</td>
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<td>-4.90</td>
<td>1.14</td>
</tr>
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<td>241Pu</td>
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<td>-4.72</td>
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<tr>
<td>237Np</td>
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<td>14.30</td>
<td>2.45</td>
</tr>
<tr>
<td>99Tc</td>
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<td>9.58</td>
<td>14.60</td>
<td>14.94</td>
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<tr>
<td>137Cs</td>
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<td>-0.38</td>
<td>3.90</td>
<td>0.70</td>
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</tbody>
</table>

### Case D

<table>
<thead>
<tr>
<th>Isotope</th>
<th>MCNP6</th>
<th>MCNPx</th>
<th>SCALE</th>
<th>MONTEBURNS</th>
</tr>
</thead>
<tbody>
<tr>
<td>235U</td>
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</tr>
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<td>236U</td>
<td>0.17</td>
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<td>238U</td>
<td>-0.73</td>
<td>-0.73</td>
<td>-0.80</td>
<td>-0.89</td>
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<tr>
<td>238Pu</td>
<td>-8.58</td>
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<td>239Pu</td>
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<td>240Pu</td>
<td>1.32</td>
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<td>2.71</td>
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<td>237Np</td>
<td>1.58</td>
<td>3.08</td>
<td>18.40</td>
<td>7.91</td>
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<tr>
<td>99Tc</td>
<td>7.79</td>
<td>5.53</td>
<td>11.20</td>
<td>11.90</td>
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<tr>
<td>137Cs</td>
<td>-2.45</td>
<td>-3.09</td>
<td>1.50</td>
<td>-1.44</td>
</tr>
</tbody>
</table>
Notes on Results

- **Results**
  - No code best predicts all isotopes at all burnups
  - Creation and destruction is dictated by spectrum and geometry self-shielding; it is difficult to determine the specific reaction where the methods differ
  - The difference in data or calculation setup may be generating the largest difference

- **Conclusions on MCNP6 burnup**
  - Each actinide and Cs-137 was computed to within a few %
  - Tc-99 was computed to within 12%

- **H.B Robinson**
  - At 16-28 GWD/MTU → SCALE/SAS2H, MCNPX 2.6.0, MONTEBURNS and MCNP6 produces similar results
  - 31.66 GWD/MTU → MCNP6 produces “superior” results
Issues in Burnup

- Relies on FP data for specific systems.
  - Difficult to generalize to other systems.
- Estimate of Q value/Captured fission energy is limited by incomplete datasets.
Spontaneous Fission Rate of U-235

- “Pet Peeve”
- ENDF, SOURCES4C, CINDER use $1.05 \times 10^{-5}$ n/s-g (Branching ratio $7.2 \times 10^{-11}$)
  - Phys Rev C V.23 No. 3 (1981) p.1110
- MCNP6, Ensslin, Wikipedia use $2.99 \times 10^{-4}$ n/s-g (Branching ratio $2.0 \times 10^{-9}$)
  - Phys Rev V.86 No. 1 (1952) p.21

- These numbers differ by factor of 30!
- Why?!
Summary

- Historically MCNP used fission cross sections and (integer sampling).
- Multiple other kinds of fission data have been incorporated (multiplicity, FP distributions).
- There is a need and interest in adding more fidelity to these datasets/models.