Cross-Section Comparison for Pu-238 Production in the Advanced Test Reactor at Idaho National Laboratory

May 2023

Jill R Mitchell, Brittany Jean Grayson
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Introduction

• Qualification of Advanced Test Reactor (ATR) positions for Pu-238 production has been ongoing at INL.

• During this time, new techniques have been developed and made available for ATR experiment neutronic analysis.

• A comparative study was done using the MCNP ORIGEN Activation Analysis (MOAA) tool between ENDF/B-VII.0 and ENDF/B-VIII.0 cross-section libraries to capture the impact of the change in cross-sections on the analysis needed to qualify Pu-238 production targets.
The Pu-238 production targets used in ATR were designed by Oak Ridge National Laboratory (ORNL) and are referred to as ATR GEN 1 targets.

Each Pu-238 production target consists of a stack of cylindrical pellets, composed of 20-volume% neptunium oxide (\(\text{NpO}_2\)), 70-volume% aluminum, and 10-volume% void.
• Each ATR GEN I target contains one internal samarium spacer.

• Two targets are stacked end-to-end and placed into a basket in order to increase the number of NpO$_2$-Al pellets irradiated per cycle and to utilize the full length of the ATR.
Target Qualification

• The following codes have been used to qualify the Northeast Flux Trap (NEFT), South Flux Trap (SFT), and I positions in the ATR for Pu-238 production:
  - MCNP
  - ORIGEN2.2
  - SCALE/ORIGEN-S/OPUS

• The codes were selected based on what was available when each position was being qualified.

• Two coupling methods have been developed by INL staff to support irradiation analysis.
  - MOPY
  - MOAA

• All methods were executed using the High-Performance Computing System (HPC) located at INL.
## Cross-Section Comparison

<table>
<thead>
<tr>
<th>Cross-section libraries</th>
<th>Items of Interest</th>
<th>Tool</th>
</tr>
</thead>
<tbody>
<tr>
<td>- ENDF/B-VII.0</td>
<td>- Neutron and photon heating rates</td>
<td>- MOPY</td>
</tr>
<tr>
<td>- ENDF/B-VIII.0</td>
<td>- Average fission density</td>
<td>- MOAA</td>
</tr>
<tr>
<td></td>
<td>- Average Pu-238 assay</td>
<td></td>
</tr>
<tr>
<td></td>
<td>- Average Np conversion</td>
<td></td>
</tr>
<tr>
<td></td>
<td>- Average Pu-236 (ppm)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>- Pu-238 yield (grams)</td>
<td></td>
</tr>
</tbody>
</table>
MCNP to ORIGEN2 in Python (MOPY)

- MOPY was written using the python scripting language and was developed to manage input file generation, execute MCNP5, extract and manipulate the MCNP output, transfer the data into the ORIGEN2 input file, execute ORIGEN2, and provide updated compositions for the next MCNP transport calculation.
- MOPY has been the primary tool for ATR experiment neutronic analysis for many years.
- To complete the Pu-238 production target analysis for the NEFT qualification:
  - MOPY was run for nine timesteps to capture 65 days of irradiation.
  - Assumed a constant lobe power of 20 MW
  - Approximately 70 nuclides were tracked in MOPY.
Pu-238 Production Cross-Sections: ENDF/B-VII.0

- To perform the neutronic analysis using MOPY, the ENDF/B-VII.0 cross section library in MCNP was used along with the Neptunium (Np)-236m cross section library obtained from TENDL-2017.

- To properly track the amount of Np-236m produced from the (n,2n*) reaction, MOPY must be properly set.

- MOPY has three different treatment settings (default, zero, and ratio) for calculating the cross section that leaves a product nucleus in a metastable state, and the ratio setting was deemed most suitable for the PFS target analysis.
MCNP ORIGEN Activation Analysis (MOAA)

• MOAA is an automation tool that passes data between MCNP and the SCALE modules COUPLE, ORIGEN-S, and OPUS for depletion and activation.

• MOAA automates the calculation of the following:
  − source term (reported in grams and curies);
  − burnup (reported in %FIMA or MWd/MTU);
  − decay heat (reported in watts);
  − gamma heating (reported in W/cc);
  − neutron heating (reported in W/cc);
  − neutron flux for the MCNP cells of interest.

• To complete the Pu-238 production target analysis for the SFT qualification:
  − MOAA was run for eight timesteps to capture 60 days of irradiation.
  − Assumed a constant lobe power of 25.6 MW
Pu-238 Production Cross-Sections: ENDF/B-VIII.0

- The latest cross-section release includes many updates to the nuclear data.
- MOAA was specifically designed to use the ENDF/B-VIII.0 cross section library.
- Eliminated the need for the TENDL-2017 library to track the production of Np-236m.
- ENDF/B-VIII.0 is the preferred cross-section library for all future neutronic analysis in the ATR.
The following assumptions were used in the analysis:

1. Homogenization of internal structural parts has a negligible effect on the results.
2. Dividing the neptunium pellet active region into forty axial groups sufficiently captures the effects of the ATR axial flux profile on the neptunium pellets.
3. The SFT position in ATR is best scaled to the south lobe power.
4. The heating rates reported assumed a south lobe power of 25.6 MW.
MCNP Model

MCNP cross section of ATR.

MCNP axial view of Pu-Production targets.
Calculations

- **Core Power Calculation**
  
  \[ \text{Scaled Core Power (MW)} = \frac{\text{Expected Core Power (MW)}}{\text{Calculated Lobe Power (MW)}} \times \text{Expected Lobe Power (MW)} \]

- **Fission Density Calculation**
  
  \[ \text{FD} \left[ \frac{\text{fissions}}{\text{cm}^3} \right] = \left( \rho_{\text{initial}} \left[ \frac{\text{atoms}}{\text{barns} \cdot \text{cm}} \right] - \rho_{\text{current}} \left[ \frac{\text{atoms}}{\text{barns} \cdot \text{cm}} \right] \right) \times \frac{1 \times 10^{24} \text{barns}}{\text{cm}^2} \]

- **MCNP Heating Calculations**
  
  \[ \text{PHR}= (f6)(\text{HNF})(\text{Core Power}) \frac{W}{g} \]

- **MCNP Delayed Fission Product Heating Calculations**
  
  \[ \text{DHR}= (f6)(\text{DNF})(\text{Core Power}) \frac{W}{g} \]
Heat Generation Rates

![Heat Generation Rates Graph](image-url)
Heat Generation Rates

Summary of End of Cycle Heat Generation Rates for Pu-238 Production in the SFT.

<table>
<thead>
<tr>
<th>Cross-Section Library</th>
<th>Max (W/g)</th>
<th>Min (W/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENDF/B-VII.0</td>
<td>486.43</td>
<td>7.36</td>
</tr>
<tr>
<td>ENDF/B-VIII.0</td>
<td>513.12</td>
<td>7.52</td>
</tr>
<tr>
<td>% Difference</td>
<td>5.34%</td>
<td>2.15%</td>
</tr>
</tbody>
</table>
Plutonium-238 Production in the SFT

Pu-238 Yield (grams)

- Upper Tube 1
- Lower Tube 1
- Upper Tube 2
- Lower Tube 2
- Upper Tube 3
- Lower Tube 3
- Upper Tube 4
- Lower Tube 4
- Upper Tube 5
- Lower Tube 5
- Upper Tube 6
- Lower Tube 6
- Upper Tube 7
- Lower Tube 7

ENDF/B-VII.0  ENDF/B-VIII.0
## Plutonium-238 Production in the SFT

Estimated Peak Pu-238 Yield in the SFT using ENDF/B-VII.0 cross-sections after 65 days of irradiation.

<table>
<thead>
<tr>
<th>Target</th>
<th>Average Fission Density (fissions/cc)</th>
<th>Average Pu-238 Assay</th>
<th>Average Pu-238 Content (ppm)</th>
<th>Pu-238 Yield (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upper Tube 1</td>
<td>1.28E+20</td>
<td>86.0%</td>
<td>3.30</td>
<td>3.86</td>
</tr>
<tr>
<td>Lower Tube 1</td>
<td>2.32E+20</td>
<td>80.7%</td>
<td>3.33</td>
<td>5.10</td>
</tr>
<tr>
<td>Upper Tube 2</td>
<td>1.25E+20</td>
<td>86.0%</td>
<td>3.16</td>
<td>3.82</td>
</tr>
<tr>
<td>Lower Tube 2</td>
<td>2.27E+20</td>
<td>80.8%</td>
<td>3.22</td>
<td>5.06</td>
</tr>
<tr>
<td>Upper Tube 3</td>
<td>1.25E+20</td>
<td>85.9%</td>
<td>2.88</td>
<td>3.78</td>
</tr>
<tr>
<td>Lower Tube 3</td>
<td>2.27E+20</td>
<td>80.6%</td>
<td>2.94</td>
<td>5.01</td>
</tr>
<tr>
<td>Upper Tube 4</td>
<td>1.27E+20</td>
<td>85.7%</td>
<td>2.64</td>
<td>3.77</td>
</tr>
<tr>
<td>Lower Tube 4</td>
<td>2.31E+20</td>
<td>80.3%</td>
<td>2.76</td>
<td>4.99</td>
</tr>
<tr>
<td>Upper Tube 5</td>
<td>1.27E+20</td>
<td>85.8%</td>
<td>2.86</td>
<td>3.81</td>
</tr>
<tr>
<td>Lower Tube 5</td>
<td>2.32E+20</td>
<td>80.4%</td>
<td>2.95</td>
<td>5.03</td>
</tr>
<tr>
<td>Upper Tube 6</td>
<td>1.28E+20</td>
<td>85.9%</td>
<td>3.19</td>
<td>3.85</td>
</tr>
<tr>
<td>Lower Tube 6</td>
<td>2.32E+20</td>
<td>80.6%</td>
<td>3.22</td>
<td>5.08</td>
</tr>
<tr>
<td>Upper Tube 7</td>
<td>1.10E+20</td>
<td>86.6%</td>
<td>3.12</td>
<td>3.71</td>
</tr>
<tr>
<td>Lower Tube 7</td>
<td>2.00E+20</td>
<td>81.7%</td>
<td>3.23</td>
<td>4.91</td>
</tr>
<tr>
<td>Total (g):</td>
<td></td>
<td></td>
<td></td>
<td>61.78</td>
</tr>
<tr>
<td>Max</td>
<td>2.32E+20</td>
<td>86.6%</td>
<td>3.33</td>
<td>5.10</td>
</tr>
<tr>
<td>Min</td>
<td>1.10E+20</td>
<td>80.3%</td>
<td>2.64</td>
<td>3.71</td>
</tr>
<tr>
<td>Average</td>
<td>1.75E+20</td>
<td>83.4%</td>
<td>3.06</td>
<td>4.41</td>
</tr>
</tbody>
</table>

*actual production values may vary

Estimated Peak Pu-238 Yield in the SFT using ENDF/B-VIII.0 cross-sections after 65 days of irradiation.

<table>
<thead>
<tr>
<th>Target</th>
<th>Average Fission Density (fissions/cc)</th>
<th>Average Pu-238 Assay</th>
<th>Average Pu-238 Content (ppm)</th>
<th>Pu-238 Yield (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upper Tube 1</td>
<td>1.24E+20</td>
<td>86.1%</td>
<td>3.43</td>
<td>3.83</td>
</tr>
<tr>
<td>Lower Tube 1</td>
<td>2.27E+20</td>
<td>80.8%</td>
<td>3.46</td>
<td>5.07</td>
</tr>
<tr>
<td>Upper Tube 2</td>
<td>1.22E+20</td>
<td>86.2%</td>
<td>3.27</td>
<td>3.79</td>
</tr>
<tr>
<td>Lower Tube 2</td>
<td>2.22E+20</td>
<td>80.9%</td>
<td>3.35</td>
<td>5.03</td>
</tr>
<tr>
<td>Upper Tube 3</td>
<td>1.21E+20</td>
<td>86.0%</td>
<td>3.02</td>
<td>3.75</td>
</tr>
<tr>
<td>Lower Tube 3</td>
<td>2.22E+20</td>
<td>80.7%</td>
<td>3.08</td>
<td>4.98</td>
</tr>
<tr>
<td>Upper Tube 4</td>
<td>1.23E+20</td>
<td>85.9%</td>
<td>2.75</td>
<td>3.74</td>
</tr>
<tr>
<td>Lower Tube 4</td>
<td>2.26E+20</td>
<td>80.4%</td>
<td>2.86</td>
<td>4.96</td>
</tr>
<tr>
<td>Upper Tube 5</td>
<td>1.24E+20</td>
<td>85.9%</td>
<td>2.96</td>
<td>3.77</td>
</tr>
<tr>
<td>Lower Tube 5</td>
<td>2.27E+20</td>
<td>80.5%</td>
<td>3.05</td>
<td>5.01</td>
</tr>
<tr>
<td>Upper Tube 6</td>
<td>1.24E+20</td>
<td>86.1%</td>
<td>3.28</td>
<td>3.82</td>
</tr>
<tr>
<td>Lower Tube 6</td>
<td>2.27E+20</td>
<td>80.7%</td>
<td>3.33</td>
<td>5.06</td>
</tr>
<tr>
<td>Upper Tube 7</td>
<td>1.07E+20</td>
<td>86.8%</td>
<td>3.26</td>
<td>3.68</td>
</tr>
<tr>
<td>Lower Tube 7</td>
<td>1.95E+20</td>
<td>81.8%</td>
<td>3.37</td>
<td>4.88</td>
</tr>
<tr>
<td>Total (g):</td>
<td></td>
<td></td>
<td></td>
<td>61.36</td>
</tr>
<tr>
<td>Max</td>
<td>2.27E+20</td>
<td>86.8%</td>
<td>3.46</td>
<td>5.07</td>
</tr>
<tr>
<td>Min</td>
<td>1.07E+20</td>
<td>80.4%</td>
<td>2.75</td>
<td>3.68</td>
</tr>
<tr>
<td>Average</td>
<td>1.71E+20</td>
<td>83.5%</td>
<td>3.18</td>
<td>4.38</td>
</tr>
</tbody>
</table>

*actual production values may vary
Conclusions

• To support irradiation of the ATR GEN 1 targets in multiple ATR positions, multiple analyses were completed using the python-based codes, MOPY and MOAA.

• MOPY was written using the python scripting language and developed to manage input file generation, execute MCNP5, extract and manipulate the MCNP output, transfer the data into the ORIGEN2 input file, and execute ORIGEN2.

• MOAA is a python automation tool that passes data between MCNP and the SCALE modules COUPLE, ORIGEN-S, and OPUS for depletion and activation.

• All comparisons were done assuming the ATR GEN I targets were located in the SFT of the ATR.

• The initial differences are acceptable, and work is ongoing on the application of ENDF/B-VIII.0 into the remaining safety analysis.
Acknowledgments

• Multiple INL staff members contributed to the development of the MOPY and MOAA tools.

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References

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