Application of ADVANTG with MCNP to Provide Reduced Uncertainties in Isotopic Production Rates

Joel M. Risner
RNSD / Radiation Transport

David Chandler
RRD / Nuclear Safety and Experiment Analysis

Oak Ridge National Laboratory
Oak Ridge, TN, USA
Background and Objectives

• Isotopic production and decay calculations are often performed using the ORIGEN code, with flux data supplied by a radiation transport code such as MCNP.

• ORIGEN calculations are based on one-group cross-section data. For fairly ‘typical’ calculations (i.e., standard PWR designs), there are one-group ORIGEN activation/decay libraries that can be used directly. For more general analyses, the COUPLE code is used to collapse multigroup data (e.g., 238-group activation data) into a one-group ORIGEN library.

• When COUPLE is used, the calculated neutron flux is ‘binned’ into an appropriate group structure and then used to weight the multigroup activation data.
Background and Objectives

- For stochastic neutron flux calculations (such as MCNP), the calculational uncertainty in the flux spectrum can be large in some groups. This is particularly notable at high neutron energies for fission reactors due to the rapidly decreasing high-energy ‘tail’ of the fission spectrum.

- For isotopes that are produced by high-energy threshold reactions, the uncertainty in the flux spectrum will, of course, lead to uncertainties in the isotope production rate calculation. We can determine the effect of the spectrum uncertainty on the isotopic production rate using the SAMPLER code, which runs a series of COUPLE/ORIGEN calculations by sampling the calculated mean and standard deviation for each energy group.
• How can we reduce the Monte Carlo calculational uncertainty and hence improve our isotopic production estimates? The simplest approaches are, of course, to increase the number of particle histories or to apply variance reduction methods.
Background

• ORNL has pioneered the development and application of hybrid deterministic/stochastic transport methods, which utilize ‘moderate fidelity’ discrete ordinates transport calculations to generate variance reduction parameters (weight windows and consistently biased sources) that can significantly accelerate Monte Carlo solutions, and can enable solutions that were not previously achievable.

• We have incorporated this hybrid methodology into the SCALE MAVRIC sequence (which employs the Monaco Monte Carlo code) and into ADVANTG, which generates weight windows and biased sources for MCNP.
## Hybrid Transport Methods

<table>
<thead>
<tr>
<th>Monte Carlo</th>
<th>Deterministic</th>
</tr>
</thead>
<tbody>
<tr>
<td>+ Combinatorial geometry</td>
<td>+ Fast convergence</td>
</tr>
<tr>
<td>+ Point-wise cross section data</td>
<td>+ Global solutions</td>
</tr>
<tr>
<td>+ Unbiased estimates</td>
<td></td>
</tr>
<tr>
<td>+ Easy to use</td>
<td></td>
</tr>
</tbody>
</table>

**RETAI N / ENHANCE**

**MINIMIZE**

- Slow convergence
- Results at tally locations only
- Memory requirements
- Error analysis needed
- Expertise generally required
Particle Importance

\[ \phi^+(\vec{r}) = \text{Expected score of a unit-weight particle emitted at } \vec{r} \]

**Properties**

- Independent of the source
- Induced by and has same units as the tally
- Solution of an adjoint transport equation

† Very useful in Monte Carlo simulations
† Deterministic methods can calculate \( \phi^+(\vec{r}, E) \) efficiently
Using an Importance Map: The Weight-Window Technique

- **Split** particles with weights above the window
- **Take no action** for particles within the window
- **Roulette** particles below the window
Consistent Adjoint Driven Importance Sampling (CADIS)

- Weight windows/biased source with CADIS
  - Calculate adjoint fluxes from an adjoint source at a detector location
    \[ q^+ (\vec{r}, E) = \sigma_d (\vec{r}, E) \]
  - Estimate the response
    \[ R = \int\int \phi^+ (\vec{r}, E) q(\vec{r}, E) d\vec{r} dE \]
  - Create an importance map
    \[ \bar{w}(\vec{r}, E) = \frac{R}{\phi^+ (\vec{r}, E)} \]
  - ... and a consistently biased source
    \[ \hat{q}(\vec{r}, E) = \frac{1}{R} q(\vec{r}, E) \phi^+ (\vec{r}, E) \]
  - Run the forward Monte Carlo
Forward-Weighted CADIS (FW-CADIS)

- Perform a forward discrete ordinates calculation
- Estimate the responses $R(r,E)$ everywhere
- Construct the CADIS adjoint source at all ‘detector locations’ - weight the source strength by $1/R(r,E)$

- Perform an adjoint discrete ordinates calculation
- Create the weight windows and biased source (as with CADIS)
- Perform the Monte Carlo calculation
How does ADVANTG work?

**Discretize**
MCNP model geometry, source, and tallies

**Drive**
parallel 3-D $S_N$ calculations to estimate adjoint fluxes

**Calculate**
parameters using CADIS or FW-CADIS method

**Write**
parameters in a format directly usable by MCNP
The HFIR Core and Experimental Facilities

VXF-3

VXF-15

VXF-18
For this example we consider a NpO\(_2\)/Al target in the VXF-3 location in the outer (permanent) Be reflector. The target has a modeled volume of 0.109 cm\(^3\). Our objective is to obtain a well-converged flux spectrum in the target cell.
Base Case: MCNP kcode Calculation

- MCNP was run in kcode mode with 2000 active cycles of $5 \times 10^5$ histories per cycle ($1 \times 10^9$ total histories).
- Run time was approximately 1400 CPU hours
Base Case: MCNP kcode Calculation
Neutron Flux Spectrum in VXF-3 Lower Target

Neutron flux spectrum tallied with SCALE 238-group energy bins

Note the absence of any non-zero calculated flux for $E > 12.84$ MeV
Base Case: MCNP kcode Calculation
Neutron Flux Spectrum in VXF-3 Lower Target

Neutron flux spectrum tallied with SCALE 238-group energy bins
Base Case: MCNP kcode Calculation
Neutron Flux Spectrum in VXF-3 Lower Target

Neutron flux spectrum tallied with SCALE 238-group energy bins
Base Case: MCNP kcode Calculation
Neutron Flux Spectrum in VXF-18 Lower Target

Neutron flux spectrum tallied with SCALE 238-group energy bins

Note the absence of any non-zero calculated flux for $E > 12.84$ MeV
What’s the Impact of the Spectrum Uncertainties on Isotopic Production Predictions?

• Use the Sampler code to run 100 instances of ORIGEN. For each instance, the binned group flux data is sampled from the mean and standard deviation of the MCNP simulation.

• This provides an estimate of the uncertainty in the isotopic production rate that is due solely to uncertainty in the calculated flux spectrum. No other factors (including cross-section uncertainty) are included.
What’s the Impact of the Spectrum Uncertainties on Isotopic Production Predictions?

- Consider the lower NpO$_2$/Al target in the VXF-3 location.

For a list of 821 isotopes, 106 have standard deviations of greater than 20% due to the uncertainty in the MCNP flux tally. Many of those ‘large uncertainty’ cases are isotopes that have extremely low inventories. However, large errors exist for some important isotopes, including the following:

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Mass (g)</th>
<th>Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-236</td>
<td>8.901E-9</td>
<td>42.64%</td>
</tr>
<tr>
<td>Pu-236</td>
<td>7.645E-9</td>
<td>46.19%</td>
</tr>
<tr>
<td>Pu-241</td>
<td>3.184E-6</td>
<td>7.04%</td>
</tr>
</tbody>
</table>
How Can We Reduce the “Spectrum-Driven” Uncertainty?

• Use ADVANTG to generate weight windows and a consistently biased source for a substantial improvement in variance reduction.

• Step One: Create a fixed-source MCNP problem by tallying the fission neutron production rate from the kcode problem and using that tally data as a fixed source.

• Step Two: Run ADVANTG to generate the weight-window map and biased source.

• Step Three: Run the fixed-source MCNP with the ADVANTG variance reduction parameters.
ADVANTG Calculation

• We selected all three targets (VXF-3, VXF-15, and VXF-18) as adjoint source regions. Because we have multiple tallies (which are at substantially different locations), we used the FW-CADIS option with flux weighting.

• Computational times:
  – We used the MCNP kcode calculation to generate a mesh tally for the fixed source representation
  – The total ADVANTG run time (forward and adjoint Denovo cases) was ~50 CPU hours.

Relevant parameters:
• 47-neutron-group BUGLE-B7 cross-section library
• QR 16 quadrature
• Approximately 2 million mesh cells (155 x 155 x 85)
Weight Window Target Values at Z = 0:
BUGLE Group 4 (8.61 - 10.0 MeV)

ADVANTG calculation with:
47 neutron groups
~ 2 million cells
(155 x 155 x 85)
QR 16 quadrature
Weight Window Target Values at Z = 0: BUGLE Group 41 (10.677 – 37.267 eV)

Scale: 1.0E-05 to 1.0E+05

Scale: 1.0E-05 to 1.0
ADVANTG-Accelerated MCNP

• Using the weight window file and consistently biased source generated by ADVANTG, we ran a fixed-source MCNP calculation with 1E9 histories. Note that this is the same number of total histories as we ran with the 2000-cycle kcode calculation.

• The MCNP run time was \(~180\) CPU hours (compared to \(~1400\) CPU hours for the kcode case).

• Spectral comparisons (MCNP kcode vs MCNP/ADVANTG) are shown in the next few figures.
Neutron Spectra in the VXF-3 Lower Target: “Standard” MCNP vs ADVANTG

Note that the relative errors with the ADVANTG VR parameters are about a factor of 10 lower over much of the spectrum.
Neutron Spectra in the VXF-15 Lower Target: “Standard” MCNP vs ADVANTG

Note that the relative errors with the ADVANTG VR parameters are about a factor of 10 lower over much of the spectrum.
Neutron Spectra in the VXF-18 Lower Target: “Standard” MCNP vs ADVANTG

Note that the relative errors with the ADVANTG VR parameters are about a factor of 10 lower over much of the spectrum.
Neutron Spectra in the VXF-3 Lower Target: “Standard” MCNP vs ADVANTG

![Graph showing neutron spectra comparison between MCNP and ADVANTG](image-url)
Neutron Spectra in the VXF-3 Lower Target: “Standard” MCNP vs ADVANTG

![Graph showing neutron spectra comparison between standard MCNP and ADVANTG methods. The graph plots neutron flux per unit lethargy against neutron energy (eV).]
What Did We Gain by Using ADVANTG?

• In the original kcode calculation, there were 106 isotopes (out of a list of 821) which had standard deviations of >20% in the isotopic production rate predictions due solely to the spectral relative errors.

• Using ADVANTG we reduced the number of “poorly converged” isotope production rates from 106 to 16. Note also that the ADVANTG-accelerated MCNP calculation required only about 15% of the CPU time of the original kcode calculation.
What Did We Gain by Using ADVANTG?

• Returning to our earlier observation about uncertainties in the lower NpO$_2$/Al target in the VXF-3 location, we have the following substantial improvements in the production of key isotopes for these targets:

<table>
<thead>
<tr>
<th>Isotope</th>
<th>“Standard” MCNP</th>
<th></th>
<th>MCNP with ADVANTG</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mass (g)</td>
<td>Std. Dev.</td>
<td>Mass (g)</td>
</tr>
<tr>
<td>U-236</td>
<td>8.901E-09</td>
<td>42.64%</td>
<td>5.854E-09</td>
</tr>
<tr>
<td>Pu-236</td>
<td>7.645E-09</td>
<td>46.19%</td>
<td>4.810E-09</td>
</tr>
<tr>
<td>Pu-241</td>
<td>3.184E-06</td>
<td>7.04%</td>
<td>3.333E-06</td>
</tr>
</tbody>
</table>
Summary and Conclusions

• In previous studies we have demonstrated substantial improvements in the convergence of MCNP and MCNPX radiation transport calculations by use of the hybrid transport methodology in ADVANTG. Those studies have typically been directed toward integral responses for deep penetration problems.

• In this study we have demonstrated a significant benefit of using MCNP with ADVANTG for isotopic production calculations. While this application is not a deep penetration problem, it does require well-converged detailed neutron spectra for use with COUPLE and ORIGEN.
Summary and Conclusions

• Use of the ADVANTG-generated VR parameters reduced the uncertainty in the calculated neutron spectrum, typically by an order of magnitude, while also reducing the MCNP CPU time significantly.

• The improved spectral convergence leads to substantial reductions in the ‘flux-driven’ uncertainty in ORIGEN isotopic production rates. For the isotope production target in this example, meaningful predictions of some key isotopes would be exceedingly hard to obtain without the use of the hybrid approach.
Supplemental Slides
How does ADVANTG work?

**Discretize**
MCNP model geometry, source, and tallies

**Drive**
parallel 3-D $S_N$ calculations to estimate adjoint fluxes

**Calculate**
parameters using CADIS or FW-CADIS method

**Write**
parameters in a format directly usable by MCNP
**CADIS Methodology in MAVRIC**

- Nearly automatic – user supplies only
  - Mesh grid (coarse) for the discrete ordinates calculations
  - Adjoint source, which corresponds to the tally to optimize

<table>
<thead>
<tr>
<th>Define the adjoint source</th>
<th>$q^+ (\mathbf{r}, E) = \sigma_d (\mathbf{r}, E)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solve for the adjoint flux</td>
<td>$\phi^+ (\mathbf{r}, E)$</td>
</tr>
<tr>
<td>Estimate detector response</td>
<td>$c = \iiint q(\mathbf{r}, E) \phi^+ (\mathbf{r}, E) , d\mathbf{r} , dE$</td>
</tr>
<tr>
<td>Construct weight windows</td>
<td>$w(\mathbf{r}, E) = \frac{c}{\phi^+ (\mathbf{r}, E)}$</td>
</tr>
<tr>
<td>Construct biased source</td>
<td>$q(\mathbf{r}, E) = \frac{1}{c} q(\mathbf{r}, E) \phi^+ (\mathbf{r}, E)$</td>
</tr>
</tbody>
</table>
## FW-CADIS in MAVRIC

<table>
<thead>
<tr>
<th>Step</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Estimate the forward flux</td>
<td>$\phi(\vec{r}, E)$</td>
</tr>
<tr>
<td>Define the adjoint source</td>
<td>$q^+(\vec{r}, E) = \frac{\sigma_d(\vec{r}, E)}{\iint \sigma_d(\vec{r}, E) \phi(\vec{r}, E) d\vec{r} dE}$</td>
</tr>
<tr>
<td>Solve for the adjoint flux</td>
<td>$\phi^+(\vec{r}, E)$</td>
</tr>
<tr>
<td>Estimate &quot;detector&quot; response</td>
<td>$c = \iint q(\vec{r}, E) \phi^+(\vec{r}, E) d\vec{r} dE$</td>
</tr>
<tr>
<td>Construct weight windows</td>
<td>$\overline{w}(\vec{r}, E) = \frac{c}{\phi^+(\vec{r}, E)}$</td>
</tr>
<tr>
<td>Construct biased source</td>
<td>$\hat{q}(\vec{r}, E) = \frac{1}{c} q(\vec{r}, E) \phi^+(\vec{r}, E)$</td>
</tr>
</tbody>
</table>