Uncertainty quantification in the AGC Experiments

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INGSM-2019
Bruges, Belgium
September 16, 2019
What are we talking about?

- Nuclear graphite data not concerned with determining the uncertainty
  - Material property changes – sometimes we see uncertainty
What are we talking about?

- Nuclear graphite data not concerned with determining the uncertainty
  - Material property changes – sometimes we see uncertainty
  - Received dose – rarely (never, if I’m honest)
And why do we care?

- When do you replace the graphite?

- **Most conservative dose level**
- **More risk but Rx do operate here**
- **Highest risk**
And why do we care?

- When do you replace the graphite?
How is this applicable to you?

- Is this just an Advanced Test Reactor (ATR) problem?
- No – it is applicable to all test reactors:

<table>
<thead>
<tr>
<th>General to all reactors</th>
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</thead>
<tbody>
<tr>
<td>Fuel enrichment</td>
</tr>
<tr>
<td>Control shim angle</td>
</tr>
<tr>
<td>Uranium cross sections</td>
</tr>
<tr>
<td>Aluminum density</td>
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<tr>
<td>Beryllium density</td>
</tr>
<tr>
<td>Fuel density</td>
</tr>
<tr>
<td>Plate thickness</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>ATR specific</th>
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</thead>
<tbody>
<tr>
<td>Fuel loading/Burnup</td>
</tr>
<tr>
<td>Core configuration</td>
</tr>
<tr>
<td>Fuel experiments</td>
</tr>
</tbody>
</table>

- Estimated uncertainty
  - About 5%
- But this is 5% *per cycle*
  - Cumulative error
- Depends upon dose and dpa/cycle
  - Low dpa = minimal
  - Higher dpa = more significant
What we are doing for AGC Experiment

Objective: Radiation damage and fast fluence

- Radiation damage (e.g. in dpa) is a function of the fluence incident at a given energy; the contribution below 0.1 MeV is small.
- Damage is calculated from the neutron energy spectrum using damage cross sections calculated in the SPECTER\(^1\) code.
- So, in order to properly characterize the experiments we have a need to measure both the fast fluence and energy spectrum.
- We also want to rigorously estimate uncertainty at all stages so as to ultimately be able to put defensible error bars on dpa in the final analysis.

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Spectral Adjustment

- Ideally we would measure the received fluence using flux wires
  - Requires estimating group fluences $\varphi$ given measured cross sections, $\sigma$, and flux wire activation measurements, $a$:

$$ a_i = \sum \sigma_j^i \varphi_j $$

- Problem: there are more energy groups ($j$) than activation measurements ($i$)
  - i.e. We need more flux wires than are available

- Need some additional source of information to close the problem…
  - Best available: MCNP (but it’s a model!)

- Hence the term Spectral Adjustment: the product of our analysis is a fluence spectrum that is the result of a model, adjusted by some incomplete set of flux wire measurements

- Adjustment using STAYSL-PNNL\(^1\) code
  - Uses a least squares fitting method, accounting for uncertainty in activities, cross-sections, and MCNP spectra

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AGC-1 and AGC-2 analysis

• Both AGC-1 and AGC-2 test trains were instrumented with 26 flux wire capsules at six different heights.

• All capsules contained Fe and Nb wires; 2 of 26 additionally contained a Ti wire, which activates to $^{46}$Sc.

• AGC-1
  - Select wires measured at INL.
  - All wires subsequently measured and analyzed at PNNL.
  - Only four isotopes measured: $^{59}$Fe, $^{54}$Mn, $^{93m}$Nb, $^{94}$Nb.

• AGC-2
  - Measured and analyzed at INL.
  - Only two isotopes measured: $^{54}$Mn, $^{94}$Nb.
  - Delays between removal from ATR and disassembly/counting allowed all $^{59}$Fe to decay.
  - Counting $^{93m}$Nb requires dissolution of the wire in order to measure low energy x-ray;
    - Not performed (but capability since re-established).
**AGC-1 example**

- Sample 8F:
  - Based on five isotopes (includes $^{46}$Sc from Ti wire)
  - Fast, thermal fluences ~50% greater than MCNP values
AGC-2 example

• Sample 8H:

• This is *not* an instance of the model agreeing with measurements
• Rather, it reflects the fact that there is little actual measured data (1 thermal and 1 threshold activity) with which to adjust the spectrum, i.e.:
• The model agrees with itself!
AGC-1 numerical experiment

• Did missing $^{59}$Fe and $^{93\text{m}}$Nb affect the AGC-2 results?
• Assess by doing a simple numerical experiment with AGC-1 data:
  – Run STAYSL using all four (or five) measured isotopes
  – Run STAYSL using only two isotopes ($^{54}$Mn and $^{94}$Nb), excluding $^{59}$Fe and $^{93\text{m}}$Nb data

<table>
<thead>
<tr>
<th>Isotopes</th>
<th>dpa</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{54}$Mn, $^{94}$Nb</td>
<td>6.08</td>
</tr>
<tr>
<td>$^{54}$Mn, $^{59}$Fe, $^{94}$Nb, $^{93\text{m}}$Nb</td>
<td>7.25</td>
</tr>
<tr>
<td>$^{54}$Mn, $^{59}$Fe, $^{94}$Nb, $^{93\text{m}}$Nb, $^{46}$Sc</td>
<td>6.35</td>
</tr>
</tbody>
</table>

• Result changes with addition of data points
• Conclusion:
  – \textit{We need more data points (i.e., flux wires)}
Improving estimates of dpa and uncertainty

- Finding 1: Uncertainty dominated by assumed MCNP uncertainty (~15%), not flux wire activation uncertainty (~2-3%)
  - *Need to quantify the true MCNP uncertainty*

<table>
<thead>
<tr>
<th>STAYSL Inputs</th>
<th>Data</th>
<th>Uncertainty</th>
<th>Covariance</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCNP Spectrum</td>
<td>✓</td>
<td>Expert Judgment</td>
<td>Gaussian Model</td>
</tr>
<tr>
<td>Flux wire activities</td>
<td>✓</td>
<td>✓</td>
<td>Gaussian Model</td>
</tr>
<tr>
<td>Cross sections</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

- Finding 2: More flux wire data changes the answer
  - *Need additional flux wire measurements for future experiments*

- Finding 3: Activities of identical wires counted at INL and PNNL differed by ~15% despite “2-3%” uncertainty
  - *Need to perform a “round-robin” counting experiment to understand discrepancy*
mcACE – MCNP Uncertainty Quantification

• mcACE was developed to quantify “true” MCNP model uncertainty
  – Samples any number of uncertain input parameters, runs multiple cases, and calculates output statistics based on one of two methods:

**Total Monte Carlo (TMC):**
• Involves creating and running $N$ random inputs and then calculating output statistics using mean, var, etc. On large models this becomes computationally infeasible in terms of time.
• Agrees with deterministic treatments of UQ while taking into account non-linearities
• MCNP statistical uncertainty must be small for this to work (empirically, should be between 5-20% of total uncertainty)

**Gesellschaft für Anlagen und Reaktorsicherheit (GRS):**
• Relies on the variance of two identically distributed runs (i.e., 2 sets of MCNP runs with 2 different random number seeds) to be equal to input uncertainties.
  • Larger individual run output uncertainties is handled allowing for large speedup factors (33x for AGC)
• GRS = shorter: $N$ inputs, run 2 seeds with 66x less particles
  • $2*N*T/66$ runtime achieved via statistical methods;
  • 33x faster than TMC! ($N*T$)

mcACE – re-analysis of AGC-1

- mcACE was used with MCNP to re-analyze AGC-1
- Seven input parameters thought to be important were sampled:
  - Fuel enrichment: +/- 0.7% (spec)
  - Control shim angle: +/- 1.5% (assumed)
  - Uranium cross sections (from cross section libraries)
  - Aluminum density: 0.4% (assumed)
  - Beryllium density: 0.3% (spec)
  - Fuel density: 0.465% (spec)
  - Plate thickness: 0.1% (assumed)
- Spectrum found to be relatively insensitive to these:
  - 1-2% through most of fast spectrum
  - Increasing to ~15% from 5-20 MeV
STAYSL re-analysis of AGC-1

- STAYSL was used to perform spectral adjustment using identical flux wire data, cross sections (IRDF), and MCNP spectrum, in two ways:
  - Currently using large (~15%), assumed uncertainty on MCNP spectrum (C.1)
  - New mcACE uncertainty (mostly ~1-2%) on MCNP spectrum (C.2)

- C.2 lowers the composite uncertainty from ~6.5% to ~2.5%, but it also changes the answer: dpa for C.2 is an average of 5.6% lower than C.1

- Lower uncertainty in MCNP spectrum in C.2 gives it higher weight in the adjustment
- Flux wire measurements become unimportant by comparison in this case
- Note: We (likely) haven’t accounted for all the important sources of uncertainty in the present mcACE analysis
**Expanded flux wire set**

- In order to increase the amount of experimental data that informs these spectral adjustments, an expanded flux wire set has been identified.

- Materials that are:
  - In IRDF
  - Available (IRMM)
  - With $t_{1/2} > 1$ month

- Trial irradiation in HFIR complete
  - Awaiting measurements

- A new suite of flux wires (or subset of them)
  - Slated for inclusion in HDG-1 and future graphite irradiation experiments

<table>
<thead>
<tr>
<th>Catalog number</th>
<th>Description</th>
<th>Reaction</th>
<th>Threshold (MeV)</th>
<th>Wire diameter (mm)</th>
<th>Half-life (d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>IRMM-521 (B)</td>
<td>Ni</td>
<td>Ni58(N,P)CO58</td>
<td>0.3</td>
<td>0.5</td>
<td>70.86</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Ni60(N,P)CO60</td>
<td>3.3</td>
<td>0.5</td>
<td>1925.38</td>
</tr>
<tr>
<td>IRMM-522 (C)</td>
<td>Cu</td>
<td>CU63(N,A)CO60</td>
<td>3</td>
<td>0.5</td>
<td>1925.38</td>
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<tr>
<td>IRMM-524 (B)</td>
<td>Fe</td>
<td>FE54(N,P)MN54</td>
<td>0.8</td>
<td>0.5</td>
<td>312.00</td>
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<tr>
<td></td>
<td></td>
<td>FE54(N,A)CR51</td>
<td>1</td>
<td>0.5</td>
<td>27.70</td>
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<td></td>
<td></td>
<td>FE58(N,G)FE59</td>
<td>N/A</td>
<td>0.5</td>
<td>44.60</td>
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<tr>
<td>IRMM-525 (C)</td>
<td>Nb 19.6 ± 1.8 mg Ta kg⁻¹</td>
<td>NB93(N,N')NB93M</td>
<td>0.03</td>
<td>0.5</td>
<td>5891.48</td>
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<tr>
<td></td>
<td></td>
<td>NB93(N,G)NB94</td>
<td>N/A</td>
<td>0.5</td>
<td>7414575</td>
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<tr>
<td></td>
<td></td>
<td>TA181(N,G)TA182</td>
<td>N/A</td>
<td>0.5</td>
<td>114.43</td>
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<tr>
<td>IRMM-526 (C)</td>
<td>Nb 0.30 ± 0.09 mg Ta kg⁻¹</td>
<td>NB93(N,N')NB93M</td>
<td>0.03</td>
<td>0.5</td>
<td>5891.48</td>
</tr>
<tr>
<td></td>
<td></td>
<td>NB93(N,G)NB94</td>
<td>N/A</td>
<td>0.5</td>
<td>7414575</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TA181(N,G)TA182</td>
<td>N/A</td>
<td>0.5</td>
<td>114.43</td>
</tr>
<tr>
<td>IRMM-527R (C)</td>
<td>Al - 0.1% Co</td>
<td>CO59(N,2N)CO58</td>
<td>10.6</td>
<td>1</td>
<td>70.86</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CO59(N,G)CO60</td>
<td>N/A</td>
<td>1</td>
<td>1925.38</td>
</tr>
<tr>
<td>IRMM-531 (C)</td>
<td>Ti</td>
<td>TI46(N,P)SC46</td>
<td>2.5</td>
<td>0.5</td>
<td>83.79</td>
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<tr>
<td></td>
<td></td>
<td>TI47(N,X)SC46</td>
<td>10.8</td>
<td>0.5</td>
<td>83.79</td>
</tr>
<tr>
<td>IRMM-532 (B)</td>
<td>Al - 0.01% Co</td>
<td>CO59(N,2N)CO58</td>
<td>10.6</td>
<td>0.5</td>
<td>70.86</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CO59(N,G)CO60</td>
<td>N/A</td>
<td>0.5</td>
<td>1925.38</td>
</tr>
<tr>
<td>IRMM-533 (B)</td>
<td>Al - 0.1% Ag</td>
<td>AG109(N,G)AG110M</td>
<td>N/A</td>
<td>0.5</td>
<td>249.95</td>
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<tr>
<td>IRMM-534 (B)</td>
<td>Al - 2.0% Sc</td>
<td>SC45(N,G)SC46</td>
<td>N/A</td>
<td>0.5</td>
<td>83.79</td>
</tr>
</tbody>
</table>
Initial round-robin flux wire study - problems

- Three series of comparative counts undertaken, involving four labs:
  - INL (AL, RML, and IRC-B5), PNNL
- AGC-1: AL counts all isotopes consistently ~15% lower than PNNL
- Flux wires from AGC-3, AGR-2:
  - Differences are greater than stated uncertainty, but no trend

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Sample</th>
<th>AL</th>
<th>RML</th>
<th>PNNL</th>
<th>AL/RML ratio</th>
<th>AL/PNNL ratio</th>
<th>RML/PNNL ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mn-54</td>
<td>AGC-3: YA</td>
<td>1.34E+02</td>
<td>1.33E+02</td>
<td></td>
<td></td>
<td>90.26%</td>
<td>100.87%</td>
</tr>
<tr>
<td></td>
<td>AGC-3: R7</td>
<td>1.17E+02</td>
<td>1.05E+02</td>
<td></td>
<td>101.09%</td>
<td>99.98%</td>
<td>91.78%</td>
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<tr>
<td></td>
<td>AGC-3: DA</td>
<td>1.74E+02</td>
<td>1.74E+02</td>
<td></td>
<td>112.01%</td>
<td>102.38%</td>
<td>112.01%</td>
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<tr>
<td></td>
<td>AGR-2: BOTFW-17 (Z)</td>
<td>8.72E+01</td>
<td>9.73E+01</td>
<td>9.50E+01</td>
<td>89.64%</td>
<td>113.14%</td>
<td>89.87%</td>
</tr>
<tr>
<td>Mn-54</td>
<td>AGR-2: BOTFW-17 (Z)</td>
<td>3.01E+05</td>
<td>3.16E+05</td>
<td></td>
<td></td>
<td>95.29%</td>
<td>111.12%</td>
</tr>
<tr>
<td></td>
<td>AGR-2: BOTFW-16 (A5*)</td>
<td>1.12E+03</td>
<td>9.90E+02</td>
<td></td>
<td>102.24%</td>
<td>99.87%</td>
<td>99.87%</td>
</tr>
<tr>
<td></td>
<td>AGR-2: BOTFW-25 (4)</td>
<td>9.83E+02</td>
<td>8.85E+02</td>
<td>9.84E+02</td>
<td>111.12%</td>
<td>99.87%</td>
<td>89.87%</td>
</tr>
<tr>
<td>Co-60</td>
<td>AGR-2: BOTFW-17 (Z)</td>
<td>3.46E+00</td>
<td>3.54E+00</td>
<td></td>
<td></td>
<td>96.65%</td>
<td>105.78%</td>
</tr>
<tr>
<td></td>
<td>AGR-2: BOTFW-16 (A5*)</td>
<td>2.60E+00</td>
<td>2.54E+00</td>
<td></td>
<td>102.24%</td>
<td>97.73%</td>
<td>93.83%</td>
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<tr>
<td></td>
<td>AGR-2: BOTFW-25 (4)</td>
<td>4.97E+00</td>
<td>5.30E+00</td>
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<td>90.26%</td>
<td>97.07%</td>
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<td>Sc-46</td>
<td>AGC-3: YA</td>
<td>4.64E+01</td>
<td>4.78E+01</td>
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<td></td>
<td>96.65%</td>
<td>105.78%</td>
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<td>AGC-3: R7</td>
<td>2.60E+00</td>
<td>2.54E+00</td>
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<td>102.24%</td>
<td>97.07%</td>
<td>93.83%</td>
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<td>AGC-3: DA</td>
<td>4.97E+00</td>
<td>5.30E+00</td>
<td></td>
<td></td>
<td>96.65%</td>
<td>105.78%</td>
</tr>
</tbody>
</table>

- AGC-2: IRC-B5 counts consistently (all isotopes) ~1.9x AL values
- Desired clarity not yet achieved!
- Counting procedures to be scrutinized in FY20
Summary and conclusions

- **Minimum** dose uncertainty in material test reactors ~ 2% per cycle
  - Higher for more complex reactor designs

- In order to better quantify (and hopefully reduce) uncertainty in graphite radiation damage estimates, a multi-faceted effort is underway to better understand the models and measurements that inform this process

- mcACE uncertainty quantification tool developed to sample MCNP input uncertainties and propagate these to a “true” model uncertainty
  - Proved valuable for understanding sensitivities, but probably haven’t captured all sources of uncertainty with this analysis yet

- Need an expanded suite of flux wires to provide more activation measurements for experiments
  - Need long decay times (for ATR) of activated wires
  - HFIR trial irradiation complete. Analysis and future experiments to come

- Activation measurement uncertainties appear to be greater than previously thought based on measurements of identical wires at different labs
  - Further investigation of counting procedures is planned
STAYSL workflow

- ATR Operating History
- BCF Calculate flux history correction factors
- SigPhi Calculator Calculate corrected SigPhi estimates
- Flux Wire data
- SHIELD Perform self-shielding calculations
- STAYSL PNNL Perform neutron spectral adjustment using a least squares fitting approach
- Adjusted Fluence and Spectrum with uncertainty

- IRDF-2002
- NJOY99 Process data to obtain cross sections and covariances
- NJpp Extract cross section and covariance data to a useful format
- MCNP spectrum
AGC-1 results

Fluence > 0.11 MeV (n/cm²) vs. Height above midplane (in.)

- Channel 1
- Channel 2
- Channel 3
- Channel 4
- Channel 5
- Channel 6

MCNP

dpa vs. Height above midplane (in.)

- Channel 1
- Channel 2
- Channel 3
- Channel 4
- Channel 5
- Channel 6

MCNP
AGC-2 results

Fluence > 0.11 MeV (n/cm²)

Height above midplane (in.)

Channel 1
Channel 2
Channel 3
Channel 4
Channel 5
Channel 6
MCNP
The Total Monte Carlo Method* involves creating and running N random inputs and then calculating output statistics using mean, var, etc. On large models this becomes computationally infeasible in terms of time.

Agrees with deterministic treatments of UQ while taking into account non-linearities

Long runtime: N inputs, T runtime: N*T

Given N random runs, what is the total uncertainty?

\[
\sigma_{ob} \approx \overline{\sigma_s^2} + \sigma_i^2
\]

\[
\overline{\sigma_s^2} = \frac{1}{N} \sum_{j=1}^{N} \sigma_{s,j}^2
\]

MCNP statistical uncertainty must be small for this to work (empirically, should be between 5-20% of total uncertainty)

Given a model, where \( X \) is a model, \( Y, U \) are random \( \text{vars} \)

\[ Y = X(U) \]

The expected value and the mean are:

\[ \mu = \mathbb{E}[Y], \quad \sigma^2 = \text{Var}(\mathbb{E}[Y|U]). \]

Note also, the mean can be represented using the iterated expectations (sometimes called law of total expectation),

\[ \mu = \mathbb{E}[\mathbb{E}[Y|U]], \]

We want to know the variance of the calculation given 2 outputs that are identically distributed

\[ \text{Cov}[Y, Y'] = \mathbb{E}[YY'] - \mathbb{E}[Y]\mathbb{E}[Y'], \]

\[ \text{Def of Cov} = \mathbb{E}[\mathbb{E}[Y|U]^2] - \mathbb{E}[Y]^2, \]

\[ = \text{Var}(\mathbb{E}[Y|U]), \]