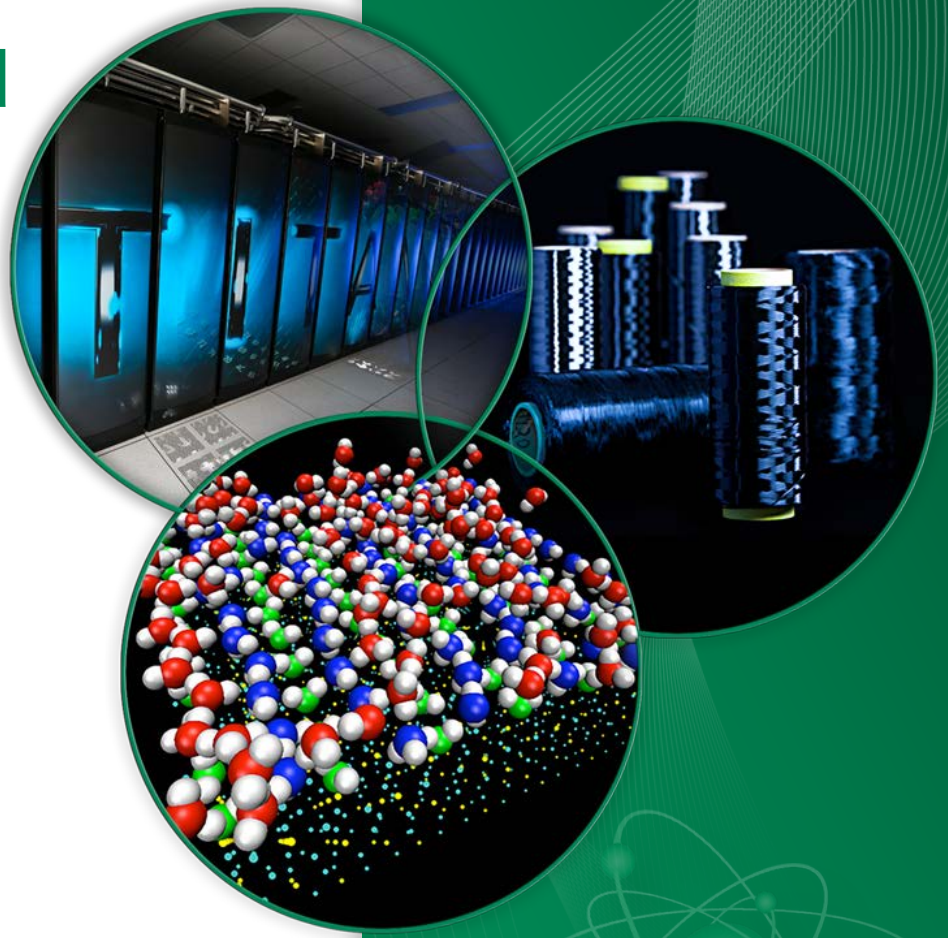
Overview of the ORNL WPNCS Efforts in Advanced Monte Carlo Techniques and Uncertainty Analysis for Criticality Safety Assessment



B.T Rearden, C. M. Perfetti, and W. J. Marshall

Nuclear Criticality Safety Program
Technical Program Review
Los Alamos, NM, March 26, 2014

Working Party on Nuclear Criticality Safety (WPNCS)

The WPNCS deals with technical and scientific issues relevant to criticality safety. Specific areas of interest include (but are not limited to) investigations of static and transient configurations encountered in the nuclear fuel cycle. These include fuel fabrication, transport and storage. The WPNCS's objectives are to:

- exchange information on national programmes in the area of criticality safety;
- guide, promote and coordinate high-priority activities of common interest to the international criticality safety community and to establish co-operation;
- monitor the progress of all activities and report to the Nuclear Science Committee (NSC);
- publish databases, handbooks and reports;
- facilitate communications within the international criticality safety community through relevant websites;
- co-ordinate the ongoing series of International Conferences on Nuclear Criticality Safety (ICNC), to be held every four years;
- co-ordinate WPNCS activities with other working groups within the NEA and in other international organisations to avoid duplication of activities; and
- provide a technical basis for the activities of other international organisations (e.g. International Organizations for Standardization (ISO), International Atomic Energy Agency (IAEA)).

Currently, the WPNCS co-ordinates 5 Expert Groups and the ICSBEP Project.

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Expert Group on Uncertainty Analysis for Criticality Safety Assessment (UACSA)

Under the guidance of the Working Party on Nuclear Criticality Safety, the Expert Group on Uncertainty Analysis for Criticality Safety Assessment was established to address issues related to Sensitivity/Uncertainty (S/U) studies for criticality safety calculations and promote exchange of information on these topics, as well as to carry out the comparison and testing of methods and computing tools for uncertainty analysis, and assist in selection and development of safe and efficient methodologies.

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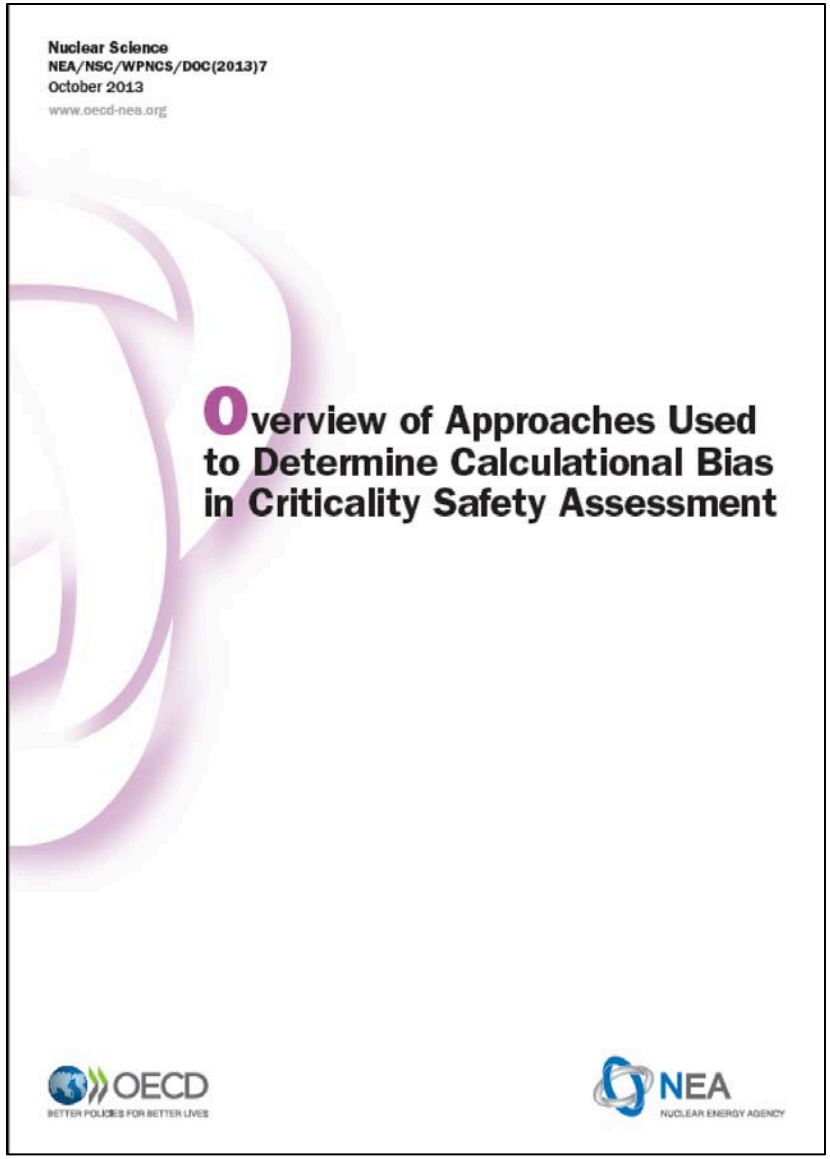
State-of-the-art Report

- Summarizes validation methods from:
  - AREVA GmbH PEPA5-G, Germany
  - Commissariat a l'Energie Atomique (CEA), France
  - E Mennerdahl Systems, EMS, Sweden
  - Institute for Physics and Power Engineering (IPPE), Russian Federation
  - Institut de Radioprotection et de Sûreté Nucléaire (IRSN), France
  - Japan Atomic Energy Agency (JAEA), Japan
  - Korean Institute of Nuclear Safety (KINS), Republic of Korea 4.8 Oak Ridge National Laboratory (ORNL), US
  - Paul Scherrer Institute (PSI), Switzerland


Nuclear Science
NEA/NSC/WPNCS/DOC(2013)7
October 2013
www.oecd-nea.org

Overview of Approaches Used to Determine Calculational Bias in Criticality Safety Assessment

OECD
BETTER POLICIES FOR BETTER LIVES

NEA
NUCLEAR ENERGY AGENCY

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UACSA Phase IV Benchmark

- Correlations between criticality safety benchmark experiments

Criticality safety benchmarks experiments as documented in the International Handbook of Evaluated Criticality Safety Benchmark Experiments of the International Criticality Safety Benchmark Evaluation Project (ICSBEP) usually belong to series of similar experimental configurations, which share certain components. As a result, it is generally not possible to treat sets of uncertain system parameters describing the respective material compositions and geometric dimensions of different benchmark experiments as mutually independent.

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Experiment Description

- Demonstration with LEU-COMP-THERM-042
- Experiments performed at PNL in 1979/1980
- Three flooded arrays of Al-clad U(2.35)O_2 powder filled rods
- Steel reflecting walls adjacent to arrays
- Controlled parameter was separation of arrays
- Various poison panels between fuel arrays
  - Stainless steel, borated stainless steel
  - Boral, Boraflex
  - Cadmium
  - Copper
  - Copper with cadmium

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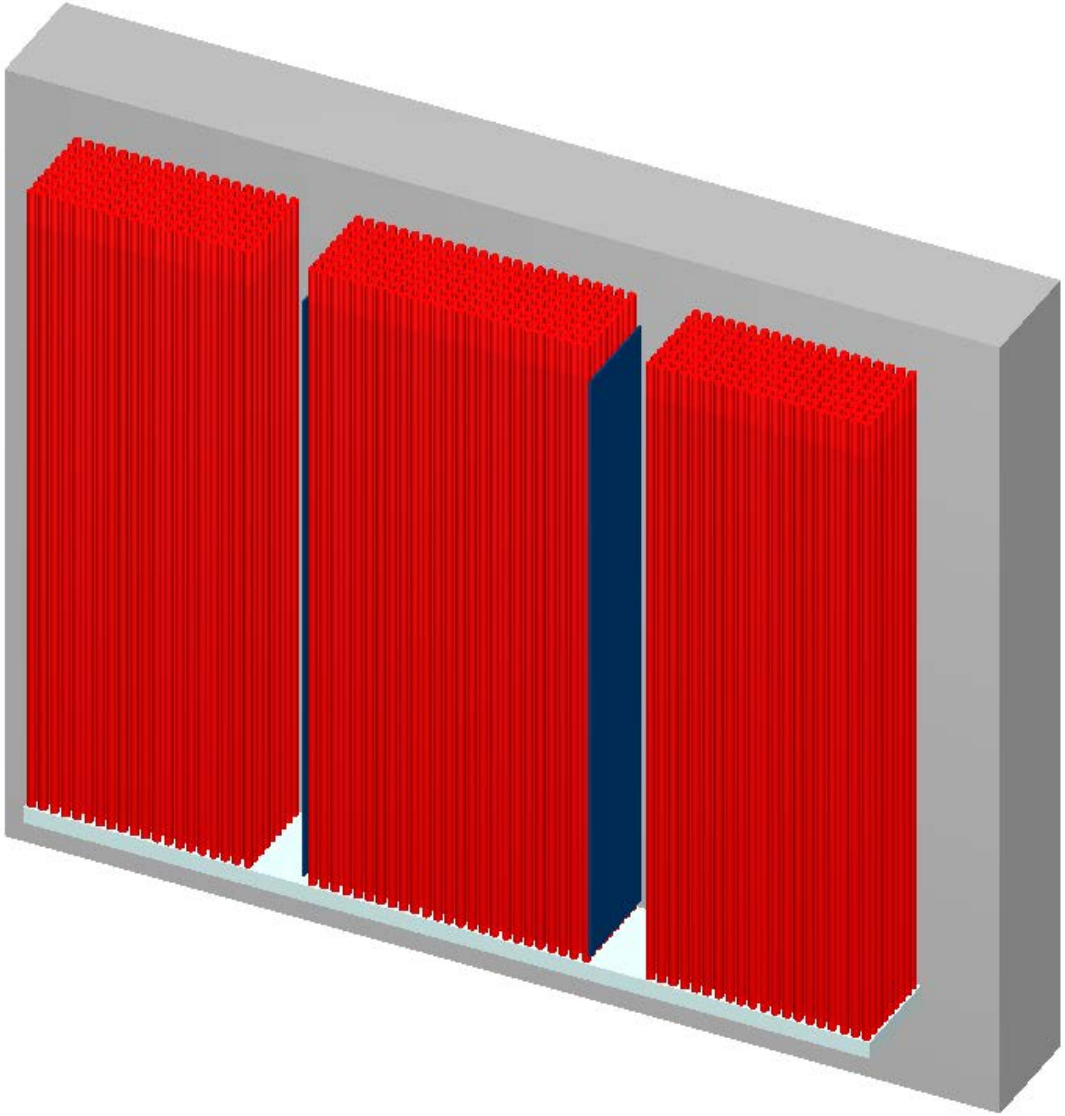
Experiment Description



KENO V.a Model

- Front half removed
- All water hidden
- Red - Cladding
- Blue - Poison panel
- Grey - Reflecting wall
- White – Lower support plate (acrylic)

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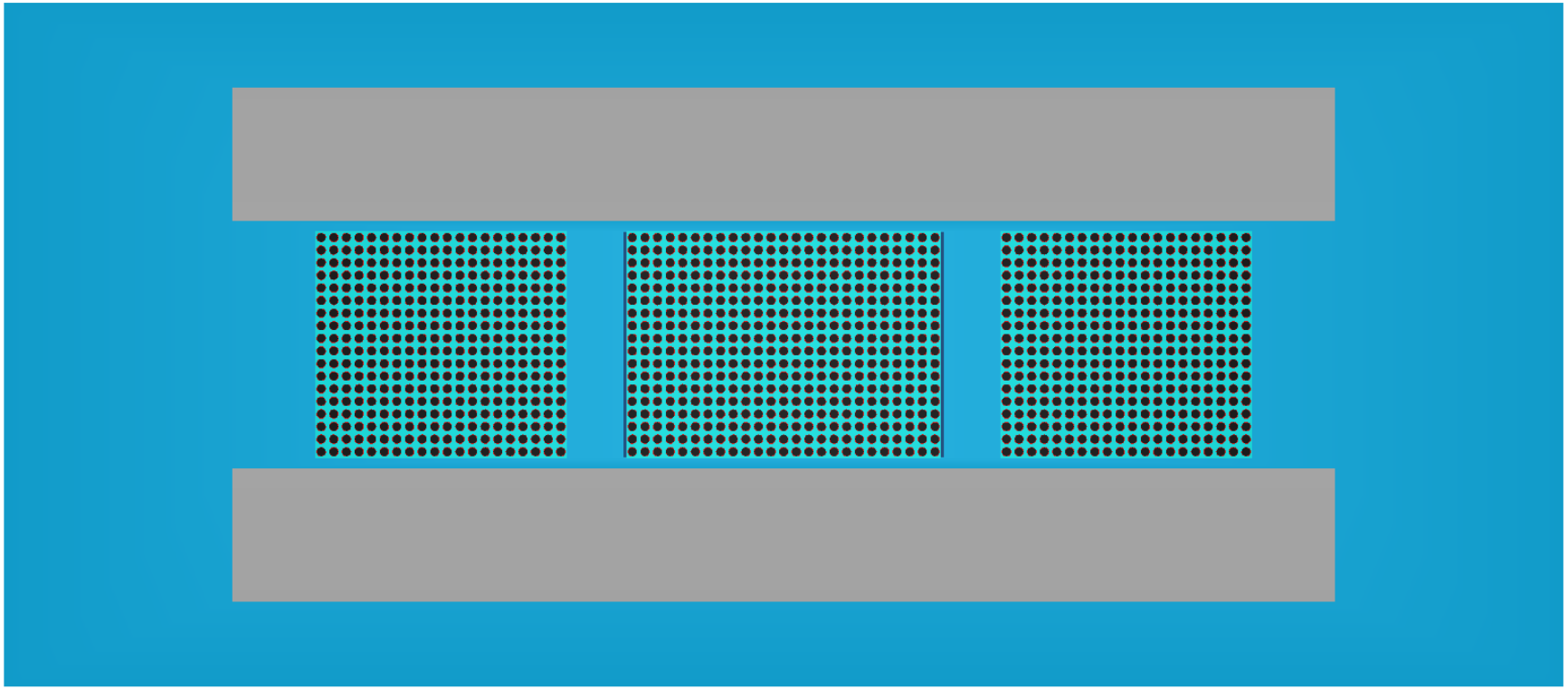
Experiment Description



Top view of model with top half removed

Blue in reflector and aqua around pins are both water with identical compositions but different cross section processing

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Methodology

- Simultaneous sampling of variable parameters, followed by calculation of correlation coefficients based on the results
- Shared sources of uncertainty are sampled the same in all appropriate cases
  - Examples: Same fuel rods, so same sampled isotopics, rod diameter, pitch in all seven cases
- Differing sources of uncertainty are sampled uniquely for each appropriate case
  - Examples: Poison panel compositions, experiment temperatures

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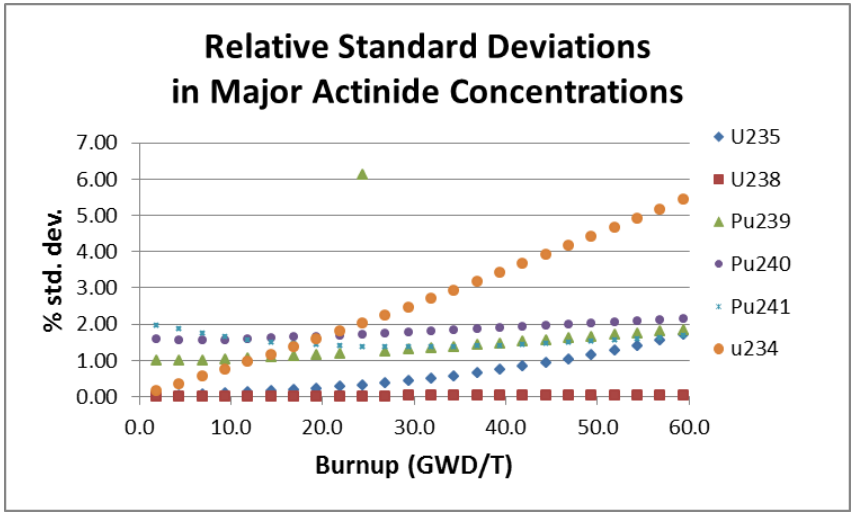
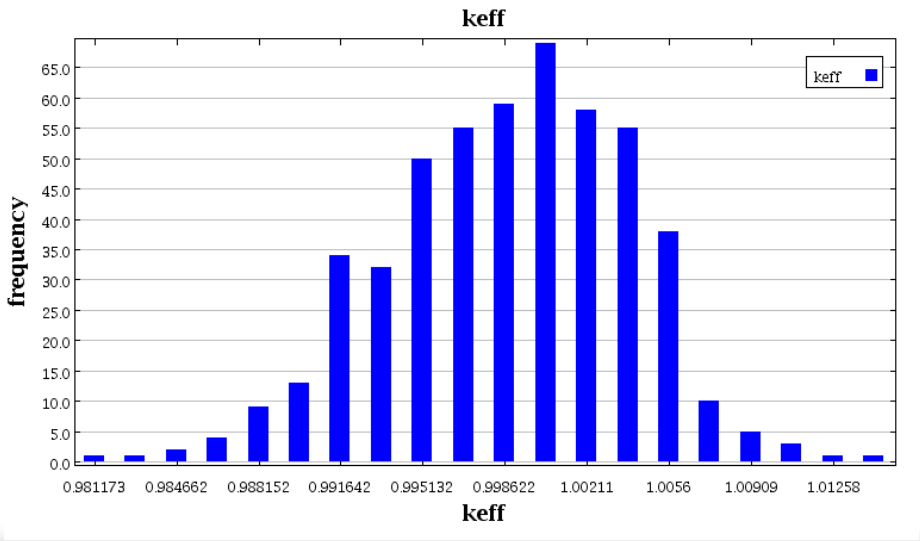
Sampler: A Module for Statistical Uncertainty Analysis with SCALE Sequences

- Sampler provides uncertainty in any computed result from any SCALE sequence due to uncertainties in:
  - neutron cross sections
  - fission yield and decay data
  - geometry and composition
- Sampler propagates uncertainties through complex analysis sequences such depletion calculations
- Correlations between systems are also computed





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Approach to Quantifying Correlations Between Uncertain Parameters Shared by Multiple Systems

- Based on empirical approach presented by Areva
  - Oliver Buss, Axel Hoefer, Jens Christian Neuber, Michael Schmid, “Hierarchical Monte-Carlo approach to bias estimation for criticality safety calculations,” PHYSOR 2012
- Generate SCALE/CSAS inputs for each model
- Identify “sets” of systems with shared uncertain parameters
- Generate single Sampler input using multiple models and multiple parameters
- Analyze results

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Methodology

- Uncertain parameters identified mostly in Section 2 of IHECSBE report, some in Section 1
- Ranges of uncertain parameters defined in Sections 1 and 2 of the report
- Distribution largely unknown
  - Some cases (e.g., pitch and enrichment) assumed normal with stated standard deviation
  - Most cases sampled from uniform (constant probability) distribution across range identified
- KENO models modified by Sampler for each perturbation of each case and run – 275 perturbations for each case

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Methodology

- Input snippets:

```
read variable[pitch_p]
  distribution = normal
    value = 0.842
    stddev = 0.0038
    minimum = 0.8306
    maximum = 0.8534
    siren="//read geometry/unit[1:4]/cuboid/Dimensions/*[1,3,7,9,13,15,19,21]"
    cases = Case1 Case2 Case3 Case4 Case5 Case6 Case7 end
end variable
'
read variable[refl_wall_t]
  distribution=constant
  minimum=17.81 maximum=17.89 value=17.85
  siren="//read geometry/unit[id='11']/cuboid/Dimensions/+y"
  cases = Case1 Case2 Case3 Case4 Case5 Case6 Case7 end
end variable
'
```

Sample half-pitch from normal distribution: 0.842 ± 0.0038, truncated at ± 3 sigma
Change +x and +y dimensions of cuboid in Units 1-4
The same value used for perturbation *n* in all cases

Sample reflecting wall thickness uniformly from 17.81 to 17.89 with nominal = 17.85
Change +y dimension in Unit 11
The same value used for perturbation *n* in all cases

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Methodology

- Input snippets:

Sample poison panel thickness uniformly from 0.289 to 0.315 with nominal = 0.302
Change +x dimension in Unit 6
Value used for perturbation *n* only in Case 1

```
read variable[pois_t1]
  distribution=constant
  minimum = 0.289 value = 0.302 maximum = 0.315
  siren="//read geometry/unit[id='6']/cuboid/Dimensions/+x/"
  cases = Case1 end
end variable
'
read variable[atom_density_u235]
  distribution = expression
  expression = "(u235_g_density * avogadro)/atomic_mass_u235"
  siren = "//read comp/u-235/aden"
  cases = Case1 Case2 Case3 Case4 Case5 Case6 Case7 end
end variable
```

Calculate ^{235}U number density based on other variables defined previously
Change number density for U-235
Value used for perturbation *n* in all cases

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Results

- Sampler calculates desired responses
  - In this case k_{eff} (and its uncertainty) and correlations among cases
- Sampler also accepts input to calculate correlation of k_{eff} in each case to various parameters (pitch, poison panel thickness, etc.)
- When multiple cases are specified, Sampler automatically calculates experimental correlations based on covariance between each pair of cases

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Results – Average k_{eff}

	Nominal case k_{eff}	KENO Uncertainty	Average k_{eff} from 275 Samples	Uncertainty in average k_{eff} of Samples	Experimental Uncertainty from Section 2
Case 1	0.99592	0.00099	0.99642	0.00270	0.0016
Case 2	0.99709	0.00098	0.99625	0.00284	0.0016
Case 3	0.99758	0.00094	0.99763	0.00277	0.0016
Case 4	0.99808	0.00099	0.99826	0.00287	0.0017
Case 5	0.99920	0.00097	0.99801	0.00276	0.0033
Case 6	0.99897	0.00085	0.99771	0.00265	0.0016
Case 7	0.99683	0.00097	0.99593	0.00278	0.0018

Individual cases run until uncertainty of 0.001 achieved in k_{eff} to manage run time for 1925 jobs

Uncertainty in average k_{eff} is not very sensitive to individual case uncertainties

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Results – Experimental Correlations

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7
Case 1	1	0.832	0.830	0.826	0.838	0.803	0.814
Case 2		1	0.831	0.831	0.854	0.810	0.829
Case 3			1	0.831	0.820	0.784	0.823
Case 4				1	0.837	0.791	0.806
Case 5					1	0.823	0.796
Case 6						1	0.803
Case 7							1

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Expert Group on Advanced Monte Carlo Techniques (AMCT)

The goal of the Expert Group is to transfer new Monte Carlo technology to criticality safety practitioners. To accomplish this several objectives/activities are required initially:

- Survey recent advances in the development of new techniques for Monte Carlo criticality analysis codes.
- Identify new techniques as high-priority for further detailed study, and solicit EG members to investigate each technique.
- For each selected technique, designated EG members will review the methodology, survey the literature, assess the verification/validation status, possibly establish benchmark tests that could be used by EG member Monte Carlo codes, and suggest guidelines for applying the new techniques to problems of importance to practitioners.
- Draft recommendations to practitioners for using the improved methodology in their work, and to guide its employment.

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Phase I Benchmark: Quantifying the Effect of Undersampling Biases in Monte Carlo Reaction Rate Tallies

Purpose:

1. To investigate how undersampling causes eigenvalue biases, reaction rate tally biases, and poor tally variance estimates.
2. To estimate the magnitude, prevalence, and impact of these biases.
3. Produce a set of recommendations and best practices for obtaining reliable Monte Carlo reaction rate estimates in models of complex systems (i.e. Monte Carlo depletion calculations).

Approach:

- Generate models of systems relevant to burnup credit applications with varying degrees of geometric and fuel isotopic complexity.
- Simulate these models using a constant number of active histories in different NPG/GEN combinations.
- Examine how eigenvalue and flux tallies change with NPG/GEN to determine the behavior of biases in these parameters.
- Repeat these simulations multiple times to obtain “true” variance estimates.

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Cases Examined

Two cases are examined in the study, each with three configurations of differing complexity:

1. PWR Core

Configuration	ID	Geometry	Isotopics	Temperature	Reaction Tally Locations
2D Quarter Core	R1	17x17 quarter core radial slice	Uniform 20 GWD/MTU with equilibrium Xenon	Reactor – Uniform Mid-Plane	Center and edge bundles
3D Core Assembly	R2	17x17 bundle in infinite lattice	18 axial zones; varying 20 GWD/MTU with equilibrium Xenon	Reactor – 18 Axial zones	Top, mid-plane, and bottom
3D Quarter Core	R3	17x17 quarter core	18 axial zones; 20 GWD/MTU with equilibrium Xenon; Uniform radially	Reactor – Uniform radially, 18 axial zones	Center and edge bundles Top, mid-plane, and bottom

2. Used Fuel Shipping Cask

Configuration	ID	Geometry	Isotopics	Temperature	Reaction Tally Locations
2D Storage Cask	S1	17x17 in cask geometry radial slice	Uniform 40 GWD/MTU with 5 year cooling time	Uniform storage temperature	Center and edge bundles
3D Cask Assembly	S2	17x17 bundle in infinite lattice	18 axial zones; 40 GWD/MTU with 5 year cooling time	Uniform storage temperature	Top, mid-plane, and bottom
3D Cask	S3	17x17 in full cask	18 axial zones; 40 GWD/MTU with 5 year cooling time; Uniform radially	Uniform storage temperature	Center and edge bundles Top, mid-plane, and bottom

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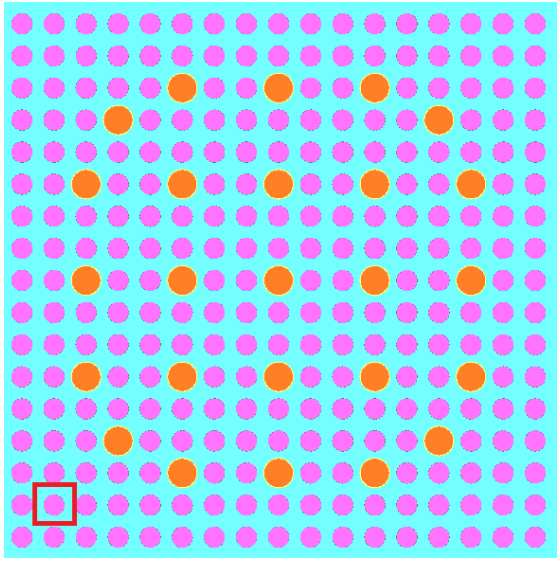
Reaction Rate Tally Locations – 2D Core (R1)

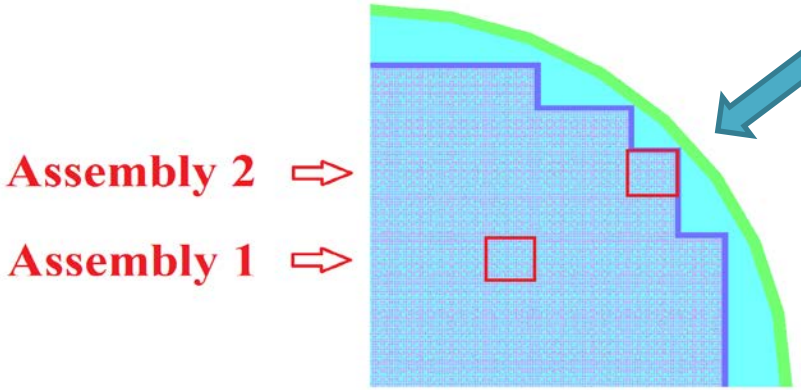
Pin 0 = All fuel pins
(Very good statistics, σ ≈ 0.001%)

Pin 1 = Fuel pin in an assembly in the middle of the quarter-core.
(Good statistics, σ ≈ 0.05%)

Pin 2 = Fuel pin in an assembly near the edge of the quarter-core.
(Poor statistics, σ ≈ 0.10%)



Fuel Pin Location in each Assembly



Assembly Locations

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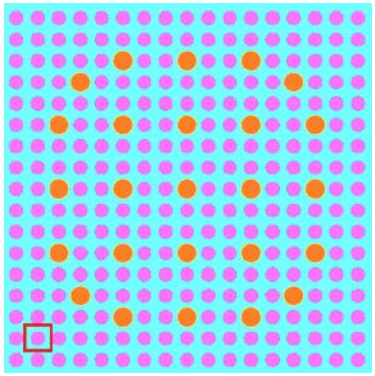
Reaction Rate Tally Locations – 3D Core Assembly (R2)

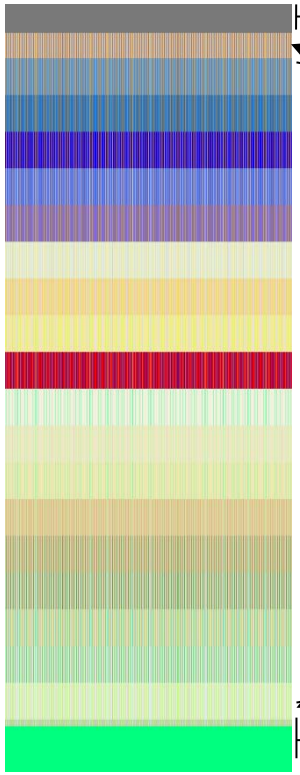
Pin 1 = Fuel pin in an axial slice 3/4'ths up the assembly.
(Good statistics, σ ≈ 0.25%)

Pin 2 = Fuel pin in an axial slice in the middle of the assembly.
(Good statistics, σ ≈ 0.15%)

Pin 3 = Fuel pin in the bottom axial slice.
(Decent statistics, σ ≈ 0.45%)



Fuel Pin Location in each Assembly



Assembly Axial Slices

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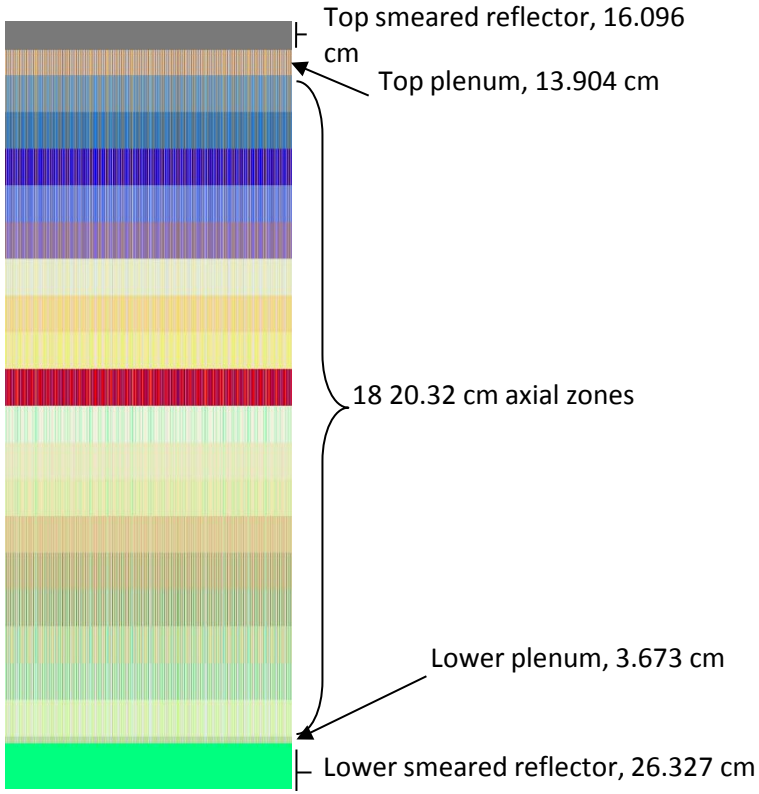
Reaction Rate Tally Locations – 3D Core (R3)

Pin 1 = Fuel pin in an assembly near the top-edge of the quarter-core.
(Good statistics, σ ≈ 1.0%)

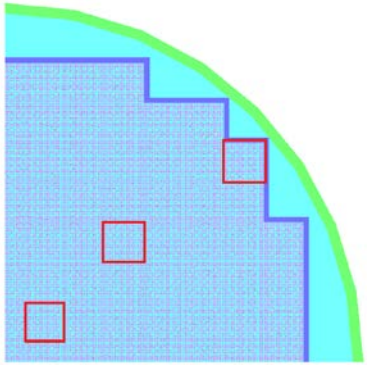
Pin 2 = Fuel pin in an assembly in the middle of the quarter-core.
(Very good statistics, σ ≈ 0.3%)

Pin 3 = Fuel pin in an assembly in the bottom-center of the quarter-core.
(Good statistics, σ ≈ 1.0%)



Assembly Axial Slices

Assembly 1 ⇨
Assembly 2 ⇨
Assembly 3 ⇨



Assembly Locations

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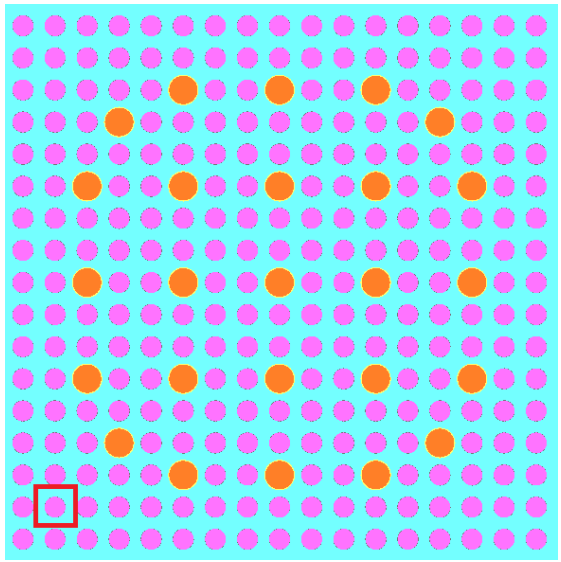
Reaction Rate Tally Locations – 2D Cask (S1)

Pin 1 = Fuel pin in an assembly near the edge of the cask.
(Good statistics, σ ≈ 0.15%)

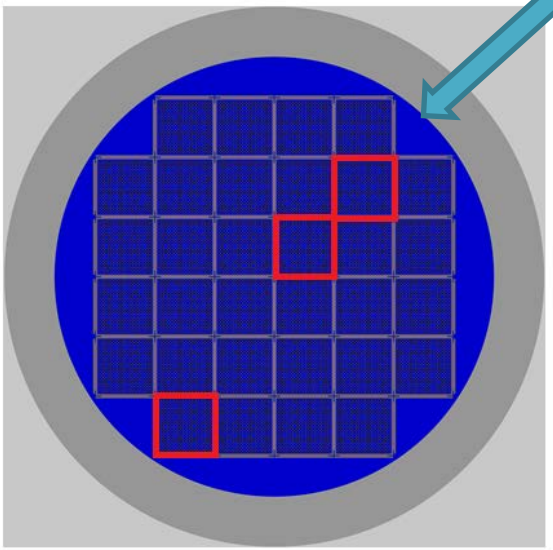
Pin 2 = Fuel pin in an assembly in the middle of the cask.
(Good statistics, σ ≈ 0.10%)

Pin 3 = Fuel pin at the edge of the cask.
(Poor statistics, σ ≈ 0.30%)



Fuel Pin Location in each Assembly

Assembly 1 ⇨
Assembly 2 ⇨
Assembly 3 ⇨



Assembly Tally Locations

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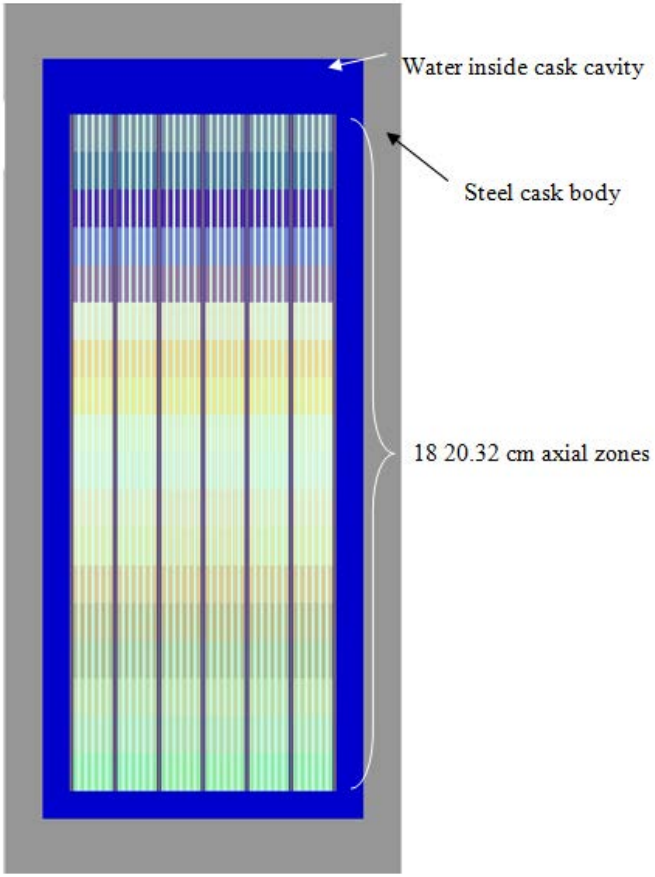
Reaction Rate Tally Locations – 3D Cask (S3)

Pin 1 = Fuel pin in an assembly near the top-edge of the cask.
(Good statistics, σ ≈ 0.25%)

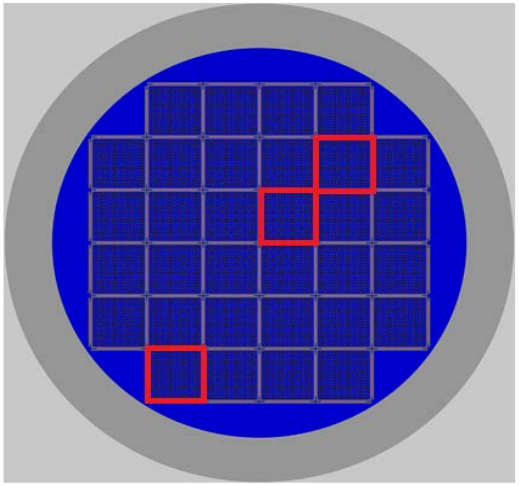
Pin 2 = Fuel pin in an assembly in the middle of the cask.
(Decent statistics, σ ≈ 1.5%)

Pin 3 = Fuel pin at the bottom-edge of the cask.
(Terrible statistics, σ ≈ 50%)



Cask Axial Slices

Assembly 1 ⇨
Assembly 2 ⇨
Assembly 3 ⇨



Assembly Tally Locations

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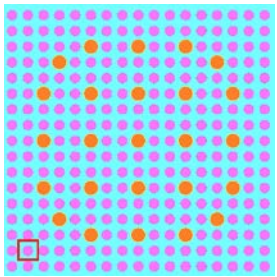
Reaction Rate Tally Locations – 3D Cask Assembly (S2)

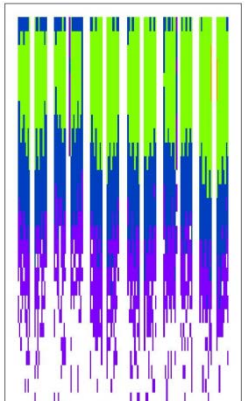
Pin 1 = Fuel pin in an axial slice 17/18ths up the assembly.
(Good statistics, σ ≈ 0.04%)

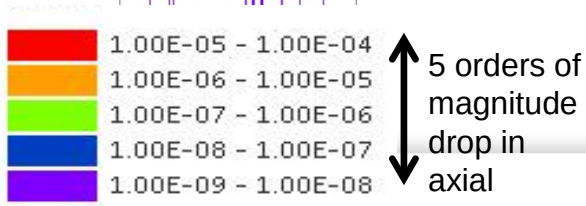
Pin 2 = Fuel pin in an axial slice in the middle of the assembly.
(Good statistics, σ ≈ 0.60%)

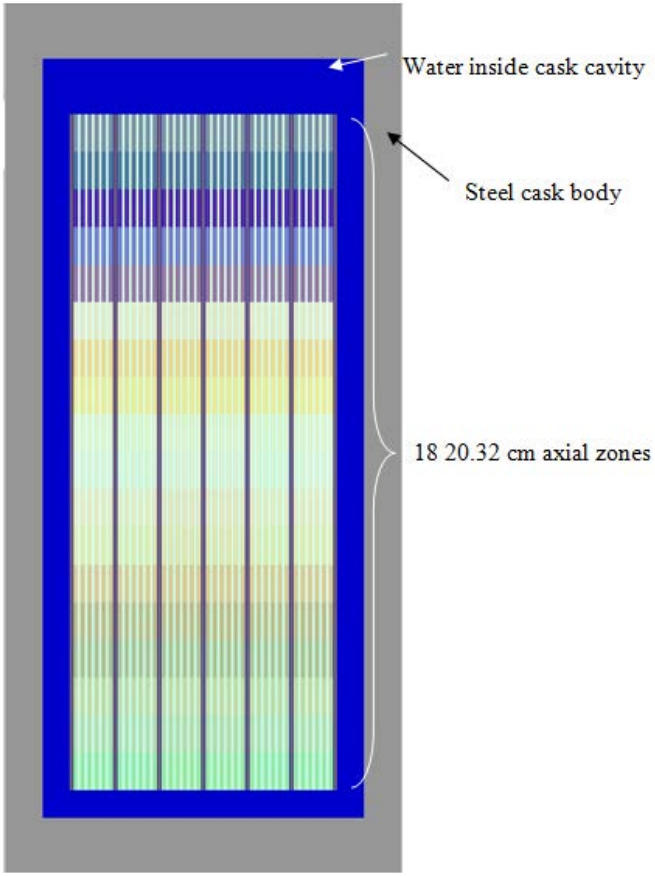
Pin 3 = Fuel pin in the second-to-bottom axial slice.
(Terrible statistics, σ ≈ 30%)



Fuel Pin Location in each Assembly







Assembly Axial Slices

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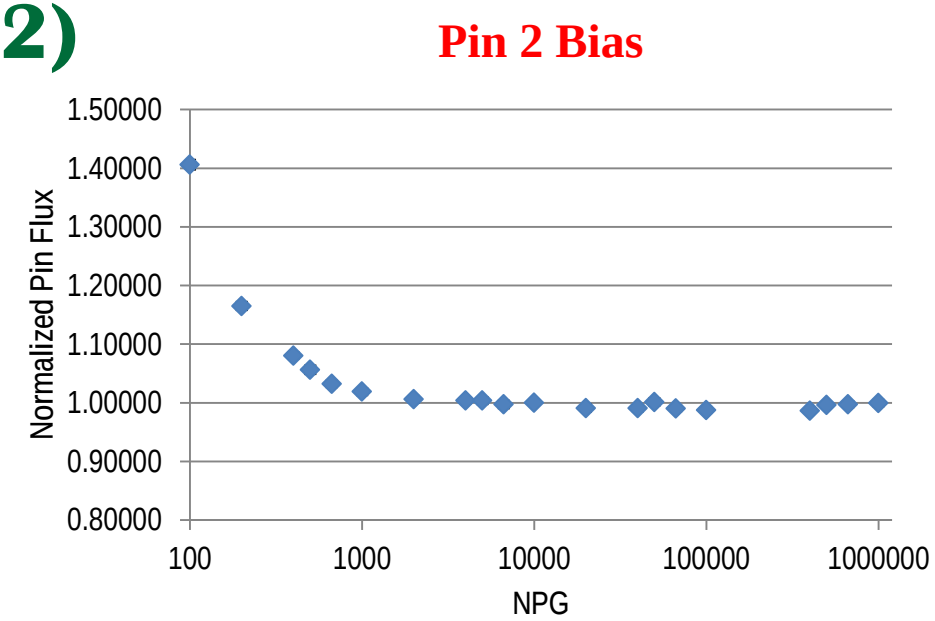
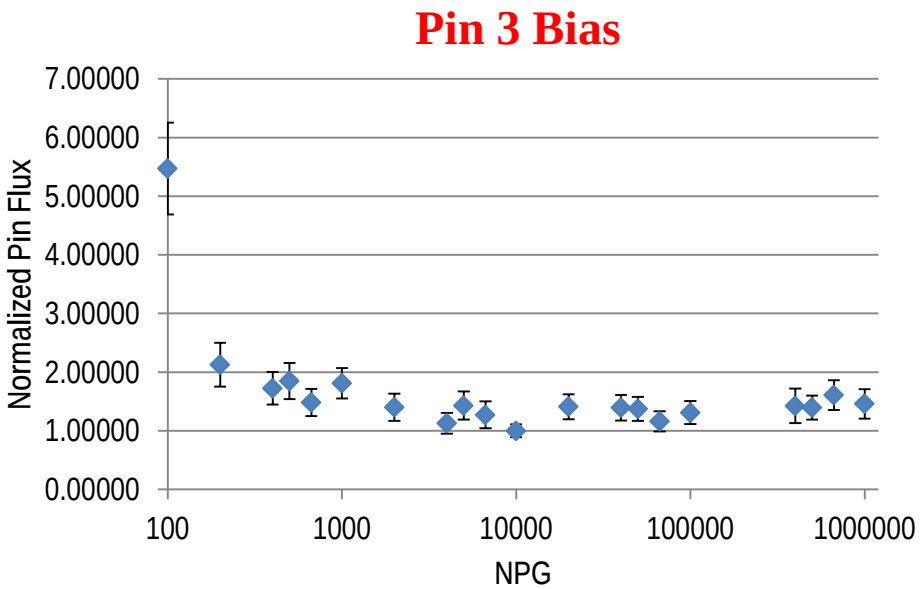
3D Cask Assembly (S2) Bias Examination

- The **Pin 2** and **Pin 3** biases were much more significant than the **Pin 1** biases.
- The **Pin 2** biases had a range of 40%, and a downward trend in the normalized pin fluxes is visible between 1,000 and 100,000 NPG.
- The **Pin 3** bias was one of the largest of any fuel pin in this study, and low NPG cases disagreed by several hundred percent.





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Continuing Work

- Large biases certainly exist when NPG is too small, and this benchmark study needs a useful way to examine the causes of these biases and should seek to develop methods/metrics for predicting when these biases will occur.
- This study tries to do too much. Having bias information for 100+ fuel pins is not useful, it's too much information to analyze. We should focus on quantifying and predicting biases for assembly fluxes or restrict our study to examine a smaller number of fuel pins.
- In its current state, this study cannot identify biases for the **3D Cask (S3)** case. It simply requires too many active histories.
- It is unclear what biases would be observed for more resolved tallies, such as:
  - Reaction-dependent tallies
  - Energy-dependent tallies
  - Reaction-/energy-/importance-dependent tallies (i.e. sensitivity coefficient tallies)

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Conclusions

- Working Party on Nuclear Criticality Safety (WPNCS)
- Expert Group on Uncertainty Analysis for Criticality Safety Assessment (UACSA)
- Expert Group on Advanced Monte Carlo Techniques (EGAMCT)
- Investigating cutting-edge issues to stay ahead of practitioner needs for NCS evaluations

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