LA-UR-11-04821

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Title: Comparison of Discrete and Continuous Thermal Neutron Scattering Cross-Section Treatments in MCNP5

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Intended for: MCNP Documentation

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Comparison of Discrete and Continuous Thermal Neutron Scattering Cross-Section Treatments in MCNP5

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August 17, 2011

Outline

- Introduction and Background
- Discrete Scattering Law Sampling Method in MCNP5
- Continuous Scattering Law Sampling Method
- Uncertainty Analysis
- Benchmark Results
- Investigation of Cases with Large Discrepancies
- Conclusions
- Future Work

Introduction and Background

- Scattering events occur in free isotopes and bound isotopes
  - These cross sections vary in the thermal energy range
  - Bound cross sections of a particular isotope vary depending on the bound target
- Upscattering and downscattering events complicate cross section determination
- Large amount of computer memory needed to store all scattering information

Introduction and Background

- Double-differential thermal neutron scattering cross section:

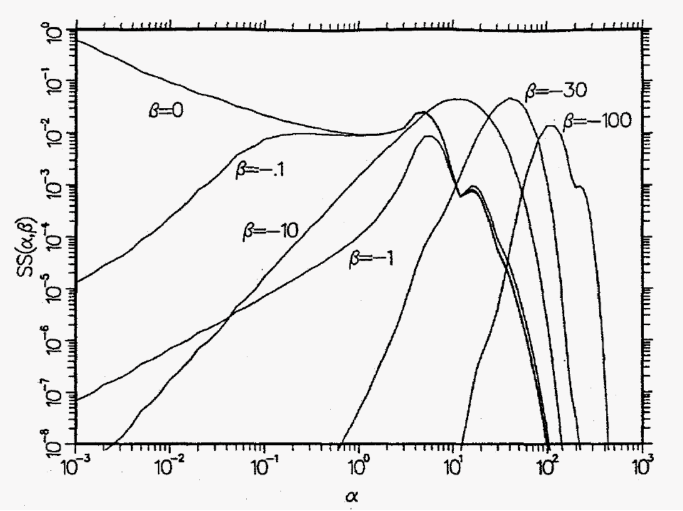
$$\sigma(E \rightarrow E', \mu) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}\exp\left(-\frac{\beta}{2}\right) S(\alpha, \beta)$$

- α and β represent, respectively, changes in momentum and energy:

$$\alpha = \frac{(\vec{p} - \vec{p'})^2}{2mAkT}$$

$$\beta = \frac{E - E'}{kT}$$

Introduction and Background



Scattering Law Sampling Method

- Method proposed by K. Cady in 1966
- Stores directly energy and angle in the form of α and β
- Double-differential cross section is converted to a function of α and β
- Sampling is performed separately for downscattering and upscattering
  - for downscattering, divide by the total downscattering cross section at the initial energy

$$f(\alpha,\beta) = \frac{\sigma(\alpha,\beta)}{\int_0^{E/kT} d\beta' \int_{\alpha_{min}}^{\alpha_{max}} d\alpha' \sigma(\alpha',\beta')} = \left[\frac{\int_{\alpha_{min}}^{\alpha_{max}} d\alpha' \sigma(\alpha',\beta')}{\int_0^{E/kT} d\beta' \int_{\alpha_{min}}^{\alpha_{max}} d\alpha' \sigma(\alpha',\beta')}\right] \cdot \left[\frac{\sigma(\alpha,\beta)}{\int_{\alpha_{min}}^{\alpha_{max}} d\alpha' \sigma(\alpha',\beta')}\right]$$

  - This is a product of two distributions

Scattering Law Sampling Method

- Given initial energy, E, sample β from the first distribution by integrating over β and setting equal to a random number:

$$\int_0^{\beta} \left[\frac{\int_{\alpha_{min}}^{\alpha_{max}} d\alpha' \sigma(\alpha', \beta')}{\int_0^{E/kT} d\beta' \int_{\alpha_{min}}^{\alpha_{max}} d\alpha' \sigma(\alpha', \beta')} \right] d\beta' = \xi$$

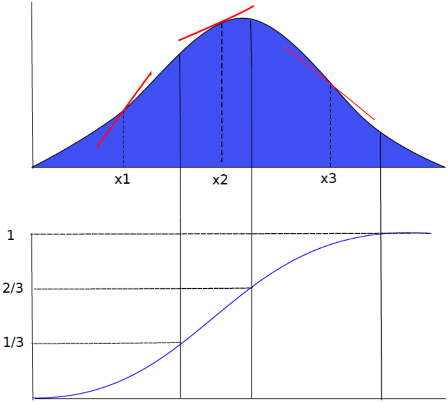
Scattering Law Sampling Method

- Given E and β from the first distribution, sample α from the second distribution by integrating over α and setting equal to a different random number:

$$\int_0^{\alpha} \left[\frac{\sigma(\alpha', \beta')}{\int_{\alpha_{min}}^{\alpha_{max}} d\alpha' \sigma(\alpha', \beta')} \right] d\alpha' = \zeta$$

- The procedure is repeated for upscattering by refining the terms using detailed balance

- Distribution function determined from Kady's method in NJOY

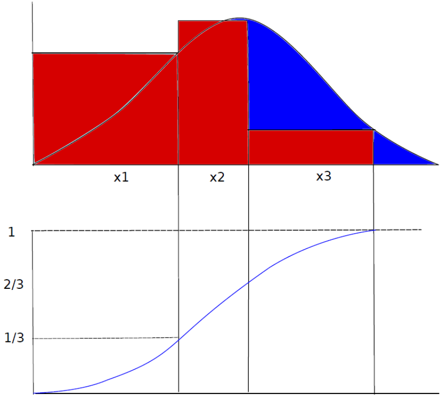


- Pick a random number ξ between 0 and 1 on cdf

For $0 < \xi < 1/3$: $x = x_1$
For $1/3 \leq \xi < 2/3$: $x = x_2$
For $2/3 \leq \xi \leq 1$: $x = x_3$

Continuous Scattering Law Sampling Method

- A more rigorous approach is suggested by Bob MacFarlane using a continuous-energy distribution
  - pdf found from sampling method proposed by Kady



- Pick a random number ξ_1 between 0 and 1 on cdf

$$
\begin{aligned}
0 < \xi_1 < 1/3: &\quad x \text{in bin } 1 \\
1/3 \leq \xi_1 < 2/3: &\quad x \text{in bin } 2 \\
2/3 \leq \xi_1 \leq 1: &\quad x \text{in bin } 3
\end{aligned}
$$

- Pick a second random number ξ_2 in the bin chosen before to determine location inside bin

Error Propagation and RMS Error

- Eigenvalues are determined for each benchmark case using both scattering treatments
- The difference in these eigenvalues is reported and uncertainty given by:

$$\delta_{\Delta k} = \sqrt{\left(\frac{\partial(\Delta k)}{\partial k_{\text{eff},d}}\right)^2 \delta^2_{k_{\text{eff},d}} + \left(\frac{\partial(\Delta k)}{\partial k_{\text{eff},c}}\right)^2 \delta^2_{k_{\text{eff},c}}}$$

- Root-Mean-Square (RMS) Error determined to compare results to the true experiment value:

$$\varepsilon = \sqrt{\sum_i (k_{\text{eff},i} - k_{\text{eff},e,i})^2}$$

t Score Correlation Test

- Used to determine if two variables follow a trend
  - Test is used to reject, within a certain confidence, the hypothesis that a trend exists
  - Each variable is assumed to follow a standard normal distribution

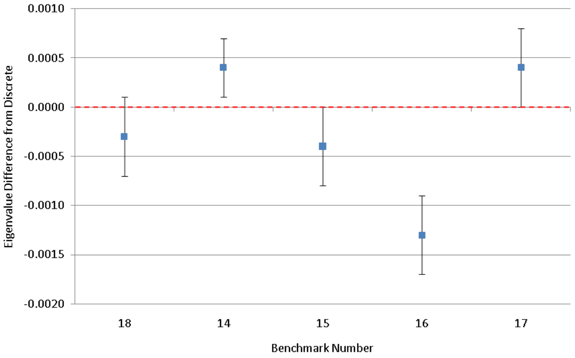
$$t = \frac{(\hat{\beta} - \beta_0)\sqrt{N-2}}{\sqrt{\frac{\sum_i \varepsilon_i^2}{\sum_i (x_i - \overline{x})^2}}}$$

t Score Correlation Test

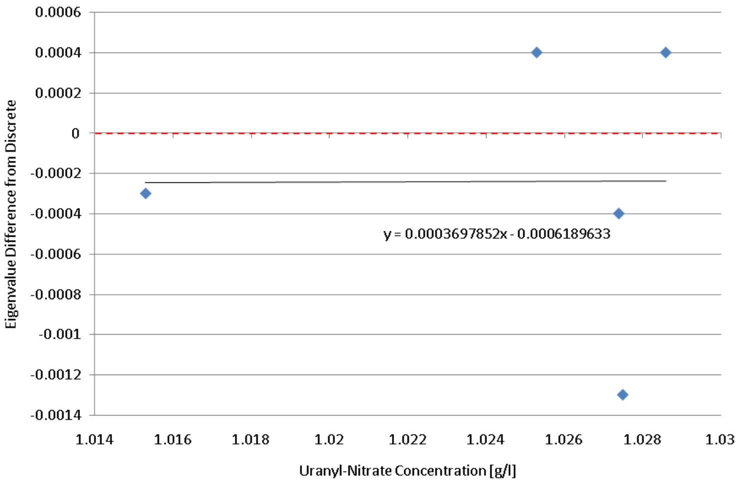
One Sided	75%	80%	85%	90%	95%	97.5%	99%	99.5%	99.75%	99.9%	99.95%
Two Sided	**50%**	**60%**	**70%**	**80%**	**90%**	**95%**	**98%**	**99%**	**99.5%**	**99.8%**	**99.9%**
1	1.000	1.376	1.963	3.078	6.314	12.71	31.82	63.66	127.3	318.3	636.6
2	0.816	1.061	1.386	1.886	2.920	4.303	6.965	9.925	14.09	22.33	31.60
3	0.765	0.978	1.250	1.638	2.353	3.182	4.541	5.841	7.453	10.21	12.92
4	0.741	0.941	1.190	1.533	2.132	2.776	3.747	4.604	5.598	7.173	8.610
5	0.727	0.920	1.156	1.476	2.015	2.571	3.365	4.032	4.773	5.893	6.869
6	0.718	0.906	1.134	1.440	1.943	2.447	3.143	3.707	4.317	5.208	5.959
7	0.711	0.896	1.119	1.415	1.895	2.365	2.998	3.499	4.029	4.785	5.408
8	0.706	0.889	1.108	1.397	1.860	2.306	2.896	3.355	3.833	4.501	5.041
9	0.703	0.883	1.100	1.383	1.833	2.262	2.821	3.250	3.690	4.297	4.781
10	0.700	0.879	1.093	1.372	1.812	2.228	2.764	3.169	3.581	4.144	4.587
11	0.697	0.876	1.088	1.363	1.796	2.201	2.718	3.106	3.497	4.025	4.437
12	0.695	0.873	1.083	1.356	1.782	2.179	2.681	3.055	3.428	3.930	4.318
13	0.694	0.870	1.079	1.350	1.771	2.160	2.650	3.012	3.372	3.852	4.221
14	0.692	0.868	1.076	1.345	1.761	2.145	2.624	2.977	3.326	3.787	4.140

U233 Benchmark Results

Case Number	Experiment k_{eff}	Discrete k_{eff}	Continuous k_{eff}	Δk from Discrete
14	1.0000(33)	1.0011(3)	1.0015(3)	0.0004(4)
15	1.0000(33)	1.0009(3)	1.0005(3)	-0.0004(4)
16	**1.0000(33)**	**1.0019(3)**	**1.0006(3)**	**-0.0013(4)**
17	1.0000(33)	0.9996(3)	1.0000(3)	0.0004(4)
18	1.0000(29)	1.0014(2)	1.0011(2)	-0.0003(3)
	RMS Error	0.00278	0.00202	
	RMS Continuous / RMS Discrete	0.72468		



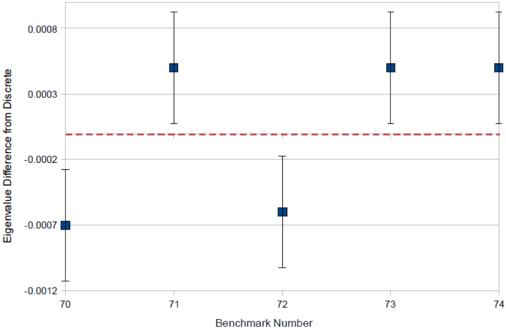
U233 Benchmark Results - t Score



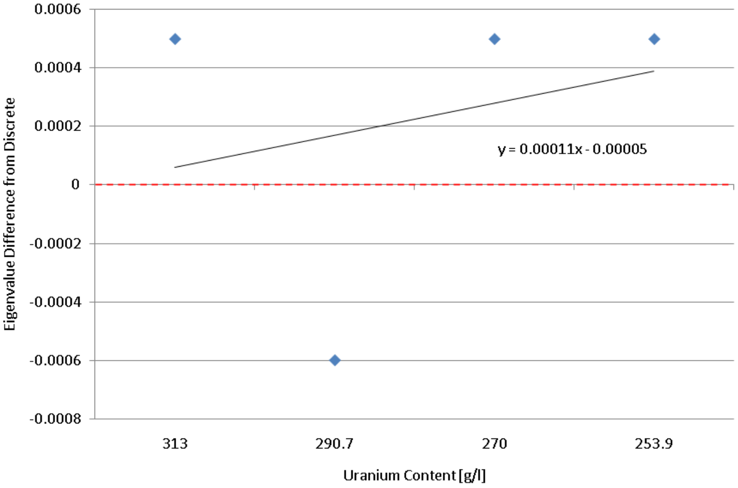
$$t \text{ Score} = 0.04$$

IEU Benchmark Results

Case Number	Experiment k_{eff}	Discrete k_{eff}	Continuous k_{eff}	Δk from Discrete
70	1.0017(44)	1.0041(3)	1.0034(3)	-0.0007(4)
71	0.9961(9)	0.9950(3)	0.9955(3)	0.0005(4)
72	0.9973(9)	0.9977(3)	0.9971(3)	-0.0006(4)
73	0.9985(10)	0.9958(3)	0.9963(3)	0.0005(4)
74	0.9988(11)	0.9986(3)	0.9991(3)	0.0005(4)
	RMS Error	0.00380	0.00287	
	RMS Continuous / RMS Discrete	0.75397		



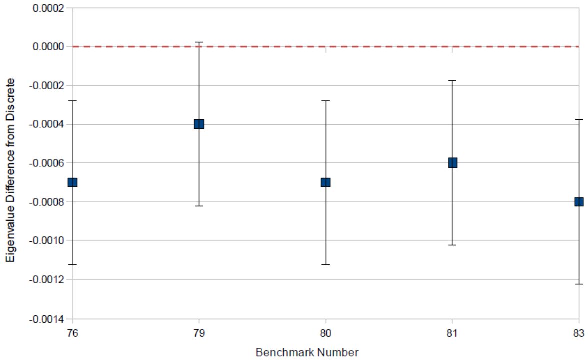
IEU Benchmark Results - t Score



t Score = 3.563

LEU Benchmark Results

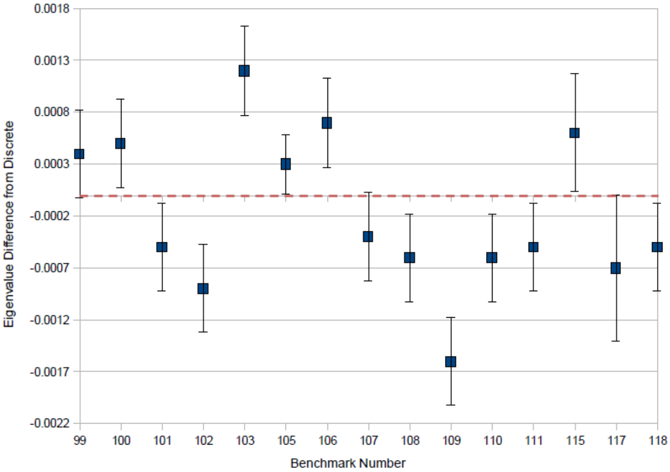
Case Number	Experiment k_{eff}	Discrete k_{eff}	Continuous k_{eff}	Δk from Discrete
76	1.0007(16)	1.0012(3)	1.0005(3)	-0.0007(4)
79	1.0007(16)	1.0003(3)	0.9999(3)	-0.0004(4)
80	1.0007(16)	1.0007(3)	1.0000(3)	-0.0007(4)
81	1.0007(16)	1.0020(3)	1.0014(3)	-0.0006(4)
83	1.0024(37)	0.9959(3)	0.9951(3)	-0.0008(4)
	RMS Error	0.00666	0.00741	
	RMS Continuous / RMS Discrete	1.11311		



Pu Benchmark Results

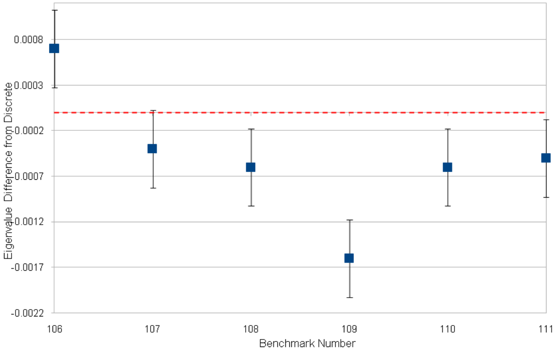
Case Number	Experiment k_{eff}	Discrete k_{eff}	Continuous k_{eff}	Δk from Discrete
99	0.9992(15)	0.9975(3)	0.9979(3)	0.0004(4)
100	1.0000(20)	1.0019(3)	1.0024(3)	0.0005(4)
101	1.0000(10)	1.0006(3)	1.0001(3)	-0.0005(4)
102	1.0000(26)	0.9931(3)	0.9922(3)	-0.0009(4)
103	1.0000(26)	1.0021(3)	1.0033(3)	0.0012(4)
105	1.0000(110)	1.0116(2)	1.0119(2)	0.0003(3)
106	1.0024(60)	1.0010(3)	1.0017(3)	0.0007(4)
107	1.0009(47)	1.0028(3)	1.0024(3)	-0.0004(4)
108	1.0042(31)	1.0032(3)	1.0026(3)	-0.0006(4)
109	**1.0024(21)**	**1.0079(3)**	**1.0063(3)**	**-0.0016(4)**
110	1.0038(25)	1.0046(3)	1.0040(3)	-0.0006(4)
111	1.0029(27)	1.0068(3)	1.0063(3)	-0.0005(4)
115	1.0000(52)	0.9996(4)	1.0002(4)	0.0006(6)
117	1.0000(65)	1.0044(5)	1.0037(5)	-0.0007(7)
118	1.0000(34)	1.0031(3)	1.0026(3)	-0.0005(4)
	RMS Error	0.01659	0.01653	
	RMS Continuous / RMS Discrete	0.99665		

Pu Benchmark Results



Pu Benchmark Results - MOX Cases

Case Number	Fuel Rods	Pitch [cm]	Soluble Boron [ppm]	Experiment k_{eff}	Discrete k_{eff}	Continuous k_{eff}	Δk from Discrete
106	469	1.77800	1.7	1.0024(60)	1.0010(3)	1.0017(3)	0.0007(4)
107	761	1.77800	687.9	1.0009(47)	1.0028(3)	1.0024(3)	-0.0004(4)
108	195	2.20914	0.9	1.0042(31)	1.0032(3)	1.0026(3)	-0.0006(4)
109	**761**	**2.20914**	**1090.4**	**1.0024(21)**	**1.0079(3)**	**1.0063(3)**	**-0.0016(4)**
110	161	2.51447	1.6	1.0038(25)	1.0046(3)	1.0040(3)	-0.0006(4)
111	689	2.51447	767.2	1.0029(27)	1.0068(3)	1.0063(3)	-0.0005(4)
	RMS Error				0.00726	0.00567	
	RMS Continuous / RMS Discrete				0.78080		



Benchmark Results

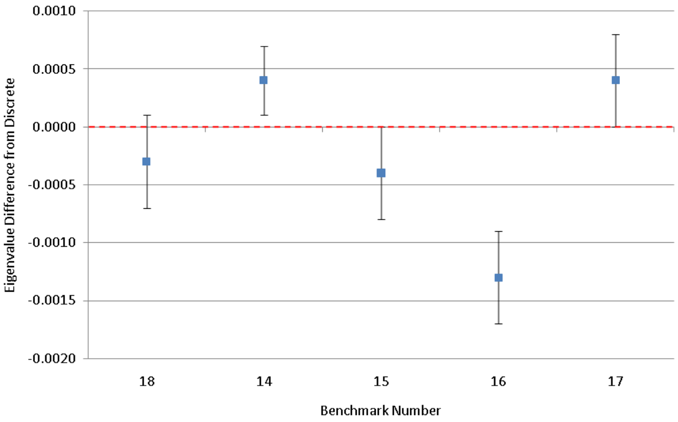
- Total RMS Error for 64 thermal scattering-treated benchmarks:

	Discrete	Continuous
Total RMS Error	0.03838	0.03857
Total RMS Continuous / Total RMS Discrete	1.00488	

- No significant difference between the two treatments
  - Large RMS differences in individual groups is a result of a small sample size where outliers dominate
- 5 of 34 cases yield an absolute eigenvalue difference between treatments of more than two standard deviations
  - 2 of these 5 cases had a difference of greater than three standard deviations

Investigation of Cases with Large Discrepancies - Case 16

- Unreflected, spherical reactor with $U(NO_3)_2$ solution in an annular shell of Aluminum with spherical source
  - Concentration of $U(NO_3)_2$ increases with benchmark number



Investigation of Cases with Large Discrepancies - Case 16

- Reran case, increasing source histories per cycle from 10,000 to 100,000

Continuous

10,000 source histories per cycle: $k_{\text{eff}} = 1.0006(3)$

100,000 source histories per cycle: $k_{\text{eff}} = 1.0009(1)$

Discrete

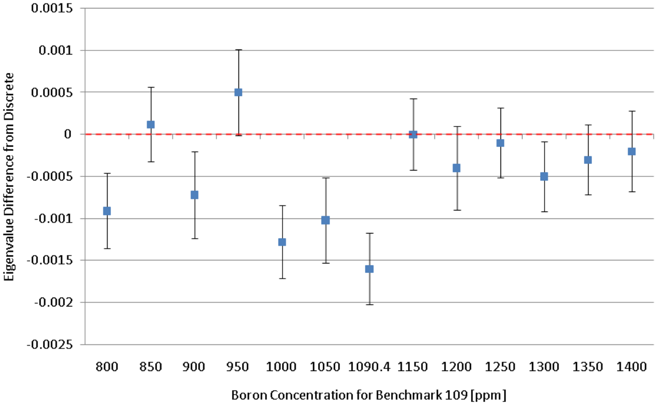
10,000 source histories per cycle: $k_{\text{eff}} = 1.0019(3)$

100,000 source histories per cycle: $k_{\text{eff}} = 1.0009(1)$

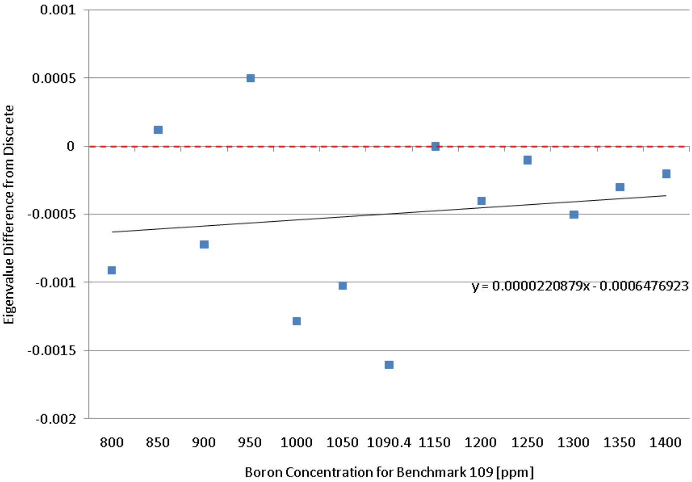
- No significant change within uncertainty for continuous

Investigation of Cases with Large Discrepancies - Case 109

- MOX lattice with fuel rods in borated water
  - displayed in order of *increasing* boron concentration



Benchmark 109 - *t* Score



$$t \text{ Score} = 23.169$$

Investigation of Cases with Large Discrepancies - Case 109

- Reran case, increasing source histories per cycle from 10,000 to 100,000

Continuous

10,000 source histories per cycle: $k_{\text{eff}} = 1.0063(3)$

100,000 source histories per cycle: $k_{\text{eff}} = 1.0069(1)$

Discrete

10,000 source histories per cycle: $k_{\text{eff}} = 1.0079(3)$

100,000 source histories per cycle: $k_{\text{eff}} = 1.0069(1)$

- The two results do not agree within their respective uncertainties, but the change is small

Conclusions

- Changes in eigenvalue between treatments are small and random and within uncertainty of measured data
- Total RMS Error is similar between treatments

Discrete: $\varepsilon = 0.03838$

Continuous: $\varepsilon = 0.03857$

- No significant change in eigenvalue expected for reactor criticality experiments
  - Using integrated values of detailed flux spectrum, so sharp edges in flux from discrete treatment are not observed
  - Experiments with a few scatters or where flux spectrum are important would require continuous-energy treatment
- Continuous treatment is a more rigorous treatment of thermal scattering, but further analysis is needed to justify a change
  - However, a change to continuous treatment does not significantly affect results for criticality experiments

Future Work

- Perform analysis on experiments where detailed thermal flux spectrum is observed
  - Change to continuous energy treatment can be made if sharp flux edges are eliminated
- Potential thesis topic: temperature-correcting thermal neutron scattering cross sections on-the-fly using scattering law in MCNP

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