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COMPARISON OF DISCRETE AND CONTINUOUS THERMAL NEUTRON SCATTERING TREATMENTS IN MCNP5

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ABSTRACT

The standard discrete thermal neutron $S(\alpha,\beta)$ scattering treatment in MCNP5 is compared with a continuous $S(\alpha,\beta)$ scattering treatment using a criticality suite of 119 benchmark cases and ENDF/B-VII.0 nuclear data. In the analysis, six bound isotopes are considered: beryllium metal, graphite, hydrogen in water, hydrogen in polyethylene, beryllium in beryllium oxide and oxygen in beryllium oxide. Overall, there are only small changes in the eigenvalue (k_{eff}) between discrete and continuous treatments. In the comparison of 64 cases that utilize $S(\alpha,\beta)$ scattering, 62 agreed at the 95% confidence level, and the 2 cases with differences larger than 3 σ agreed within 1 σ when more neutrons were run in the calculations. The results indicate that the changes in eigenvalue between continuous and discrete treatments are random, small, and well within the uncertainty of measured data for reactor criticality experiments.

Key Words: criticality, nuclear data, validation, benchmarks

1. INTRODUCTION

To provide high-fidelity modeling of thermal neutron (<4 eV) collision physics, the scattering data must account for a variety of effects having energies comparable to the neutron energy, such as thermal motion of the target nuclide, chemical binding of the target to other nuclides in a material, and crystalline effects. In this work, we compare results obtained using the traditional discrete thermal neutron $S(\alpha,\beta)$ scattering treatment provided by NJOY-MCNP [1,2] with a recently developed, more realistic, continuous $S(\alpha,\beta)$ scattering treatment using a suite of 119 ICSBEP benchmark cases [3,4] and ENDF/B-VII.0 nuclear data [5].

The traditional $S(\alpha,\beta)$ thermal scattering treatment provided by NJOY-MCNP is a complete representation of thermal neutron scattering by molecules and crystalline solids. Two processes are allowed: (1) inelastic scattering with cross section σ_{in} and a coupled energy-angle representation derived from an ENDF $S(\alpha,\beta)$ scattering law, and (2) elastic scattering with no change in the outgoing neutron energy for solids with cross section σ_{el} and an angular treatment derived from lattice parameters. The elastic scattering treatment is chosen with probability

$\sigma_{el}/(\sigma_{el} + \sigma_{in})$. This thermal scattering treatment also allows the representation of scattering by multiatomic molecules (for example, BeO). For the inelastic treatment, the distribution of secondary energies is represented by a set of equally probable final energies (typically 16 or 32) for each member of a grid of initial energies from an upper limit of typically 4 eV down to 10^{-5} eV, along with a set of angular data for each initial and final energy.

The traditional $S(\alpha,\beta)$ thermal scattering data provided by NJOY and used in MCNP represents the exit neutron energy and scattering angle pairs as discrete data. While this representation is suitable for reactor and critical experiment modeling, where integrated reaction rates are desired, it can be problematic when analyzing detailed thermal spectra (where artifacts appear in spectrum plots) or experiments where only a few scatters occur (leading to possible ray effects, especially for "broomstick" experiments) [6].

2. CONTINUOUS $S(\alpha,\beta)$ THERMAL SCATTERING TREATMENT

In the 2000s, both NJOY and MCNP5 were modified to permit the testing of a new, continuous treatment of the $S(\alpha,\beta)$ scattering data. Continuous $S(\alpha,\beta)$ scattering data for ENDF/B-VII.0 has been available on the LANL T-2 website [7]. MCNP5-1.51 [8], MCNP5-1.60 [9], and MCNP6 [10] will recognize either the old or the new $S(\alpha,\beta)$ data formats, without any additional user input.

Robert MacFarlane (the NJOY developer) modified the coding in the NJOY *aceth* module to convert the secondary energy distributions from *thermr* into PDF/CDF form and pack them into the big inelastic array in the *ace* thermal file. There is a list of incident energies, a table of the number of points in each distribution, and a table of pointers to the start of each distribution. The data for each incident energy are packed as: (E_i', PDF_i, CDF_i, $cosines_i$), (*next E_i', …*), etc. A very small amount of thinning is applied to the distributions by merging energy bins with CDF values that are less than 10^{-6}.

The *sabcol* routine in MCNP5 was modified to read in these new data and use them to drive the sampling. Given an incident energy, the coding finds the closest match in the data. The CDF table is binary searched for the random sample, and the PDF and CDF are used to linearly interpolate for an outgoing energy. The angular distribution is interpolated to this energy. Then this energy is projected up or down to correspond to the actual incident energy along lines of constant energy transfer. This tends to reproduce the sharp break near $E'=E$ and the various excitation peaks in the thermal data. For lower emitted energies (less than $0.8*E$), there is a break over to a unit-base scheme to avoid projecting to negative energies. This projection scheme is much faster than real interpolation of incident energy, but it still reproduces things well if there are enough E points in the tables. Once the final outgoing energy has been determined, cosines are sampled from the distribution at the base E and E' before projection. The cosines change more slowly than the energy distribution, so this is reasonable. The sampled discrete cosine is spread out to fill its surrounding cosine values with special measures taken at the edges.

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To use this feature, the new continuous S(α,β) datasets must be obtained from the *t2.lanl.gov* website, and version 1.51 or later of MCNP5 must be used. No changes in MCNP5 input are needed. It is imperative that users carefully check the output file to ensure that the correct data are used. Further, the continuous S(α,β) treatment has not yet been extended to cover point detector (*F5*) tallies; it should not be used in problems with *F5* neutron tallies.

3. VERIFICATION/VALIDATION TESTING

To test the effect of using discrete versus continuous S(α,β) cross sections in MCNP5, a criticality validation suite of 119 ICSBEP [4] benchmark problems developed by Mosteller [3] was used. The benchmarks are divided into five major categories based on the isotope that provides the majority of fission: Uranium-233, High-Enriched Uranium (HEU), Intermediate-Enriched Uranium (IEU), Low-Enriched Uranium (LEU) and Plutonium.

The continuous S(α, β) cross sections were specified in the MCNP inputs using an *XS* card, which reads cross-section data for the defined isotope from a specified location outside the standard *xsdir* file. The continuous S(α, β) datasets were obtained from the *t2.lanl.gov* website. These files were generated by MacFarlane using NJOY with ENDF/B-VII.0 data in October, 2007. All other materials were evaluated using the standard ENDF/B-VII.0 libraries provided with the MCNP distribution. The materials in the benchmarks that are affected by the S(α,β) treatment are hydrogen in water, hydrogen in polyethylene, beryllium metal, beryllium in beryllium oxide, oxygen in beryllium oxide, and graphite. Of the 119 benchmarks, 64 use S(α, β) thermal scattering treatments. Therefore, only these 64 benchmarks are discussed.

The 64 benchmark cases were run with MCNP5-1.60 using the traditional discrete S(α, β) treatment, and again using the continuous S(α, β). All cases were run using 100 inactive cycles, 500 additional active cycles, and 10,000 neutrons/cycle, for a total of 5 M neutrons contributing to tallies for each case. Eigenvalue uncertainties were typically 20-40 pcm (1 pcm = .00001), roughly 10 times smaller than most experimental uncertainties.

3.1. General Discussion of Results

In general, results from the discrete vs. continuous S(α, β) runs agreed within statistics in the great majority of cases: 27 of 64 cases showed differences less than 1 σ (68% confidence interval); 35 of 64 showed differences more than 1 σ, but less than 2 σ (95% confidence interval); and only 2 of 64 cases differed by more than 3 σ. A few outliers are expected with a set of 128 Monte Carlo calculations, and these were examined in detail to determine whether differences were due to underlying physics concerns or simply statistical considerations.

Results from experiment, MCNP5 analyses using the traditional discrete S(α, β) treatment, and MCNP5 analyses using the continuous S(α, β) treatment are shown in Tables I-V for each of the five benchmark categories. The "Case Numbers" listed correspond to the case numbers used in [3], and results are reported to 4 significant digits as in [3]. Two of the 64 cases showing significant differences, Case 109 and Case 16, were examined in greater detail and are discussed in Sections 3.3 and 3.4.

3.2. Metrics for Comparisons of Results

The uncertainty in the difference between discrete and continuous eigenvalues is determined using standard error propagation, where the two values are assumed to be uncorrelated. Therefore, the uncertainty in the difference of discrete and continuous eigenvalues is proportional to the square root of the sum of the squares of the individual uncertainties,

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

(1)

where $\delta_{\Delta k}$ is the standard deviation of the difference of discrete and continuous eigenvalues, $k_{\text{eff},d}$ and $k_{\text{eff},c}$ are the eigenvalue results from the discrete cross-section treatment and continuous cross-section treatment, respectively, and $\delta_{keff,d}$ and $\delta_{keff,c}$ are the standard deviations of the discrete eigenvalue and continuous eigenvalue results, respectively.

The root-mean-square error (RMS) is computed for the discrete and continuous cases, each being compared to their respective experimental result. The RMS error for the discrete treatment is given by

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

(2)

where $k_{\text{eff},d,i}$ and $k_{\text{eff},e,i}$ are the eigenvalue results for the ith benchmark for the discrete treatment and the experimental case, respectively. The RMS error for the continuous treatment is the same as Eq. (2), but with the discrete eigenvalue replaced by the continuous eigenvalue. The RMS error shows on average how far the uncertainty deviates from zero. By dividing the *Continuous RMS Error* by the *Discrete RMS Error*, an assessment of the affect of the continuous S(α,β) treatment can be made. The closer this ratio is to unity, the closer the two treatments are to one another. The RMS errors and ratios are shown in Tables I-V for each of the benchmark categories, with the overall results in Table VI.

The RMS error for the continuous S(α,β) treatment is about the same as the RMS error for the discrete treatment for the HEU and Pu categories, smaller for the U233 and IEU categories, and larger for the LEU category. Because these groups of benchmarks contain a small number of cases, the RMS error is easily inflated by large eigenvalue differences in one or two cases. Overall, the total RMS error for all 64 benchmarks is about the same for the continuous and discrete treatments. This is to be expected, since the same physical data and basic NJOY processing underlies each treatment.

Table I. U233 Benchmark Eigenvalue Results

Case Number	$S(\alpha, \beta)$-treated Isotope	Experiment k_{eff}	Discrete k_{eff}	Continuous k_{eff}	Δk from Discrete
9	Be Metal	1.0000(30)	0.9944(3)	0.9944(3)	0.0000(4)
10	Be Metal	1.0000(30)	0.9925(3)	0.9928(3)	0.0003(4)
11	H in H_2O	1.0000(83)	0.9848(5)	0.9844(5)	-0.0004(7)
12	H in H_2O / H in CH_2	1.0000(24)	1.0045(5)	1.0044(4)	-0.0001(6)
13	H in H_2O	1.0000(31)	1.0015(3)	1.0017(3)	0.0002(4)
14	H in H_2O	1.0000(33)	1.0011(3)	1.0015(3)	0.0004(4)
15	H in H_2O	1.0000(33)	1.0009(3)	1.0005(3)	-0.0004(4)
16	**H in H_2O**	**1.0000(33)**	**1.0019(3)**	**1.0006(3)**	**-0.0013(4)**
17	H in H_2O	1.0000(33)	0.9996(3)	1.0000(3)	0.0004(4)
18	H in H_2O	1.0000(29)	1.0014(2)	1.0011(2)	-0.0003(3)
	RMS Error		0.00278	0.00202	
	RMS Continuous / RMS Discrete		0.72468		

*The use of parenthesis represents standard deviation times a factor of 10^4.
For example, 0.0007(4) is equivalent to 0.0007 +/- 0.0004.

Table II. HEU Benchmark Eigenvalue Results

Case Number	$S(\alpha, \beta)$-treated Isotope	Experiment k_{eff}	Discrete k_{eff}	Continuous k_{eff}	Δk from Discrete
40	Graphite	1.0000(28)	1.0073(3)	1.0073(3)	0.0000(4)
41	O in BeO / Be in BeO	0.9992(15)	0.9955(3)	0.9955(3)	0.0000(4)
42	Be Metal	0.9992(15)	0.9957(3)	0.9951(3)	-0.0006(4)
43	H in CH_2	0.9989(15)	0.9989(3)	0.9983(3)	-0.0006(4)
44	H in CH_2	1.0000(28)	1.0008(3)	1.0005(3)	-0.0003(4)
45	H in H_2O	1.0020(10)	1.0028(3)	1.0029(3)	0.0001(4)
47	H in CH_2	1.0000(38)	1.0037(3)	1.0037(3)	0.0000(4)
49	Graphite	0.9977(8)	0.9930(3)	0.9928(3)	-0.0002(4)
50	Graphite	0.9977(8)	0.9960(3)	0.9970(3)	0.0010(4)
51	Graphite	1.0015(9)	1.0006(3)	1.0004(3)	-0.0002(4)
52	Graphite	1.0016(8)	1.0075(3)	1.0073(3)	-0.0002(4)
53	H in H_2O / H in CH_2	1.0015(28)	1.0000(4)	1.0009(4)	0.0009(6)
54	H in H_2O	1.0012(26)	0.9985(3)	0.9989(3)	0.0004(4)
55	H in H_2O	1.0007(36)	0.9975(3)	0.9973(3)	-0.0002(4)
56	H in H_2O	1.0009(36)	0.9942(3)	0.9938(3)	-0.0004(4)
57	H in H_2O	1.0003(36)	0.9957(3)	0.9959(3)	0.0002(4)
58	H in H_2O	1.0015(26)	0.9991(2)	0.9994(2)	0.0003(3)
	RMS Error		0.01604	0.01598	
	RMS Continuous / RMS Discrete		0.99630		

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Table III. IEU Benchmark Eigenvalue Results

Case Number	$S(\alpha, \beta)$-treated Isotope	Experiment k_{eff}	Discrete k_{eff}	Continuous k_{eff}	Δk from Discrete
62	Graphite	1.0000(30)	1.0075(3)	1.0075(3)	0.0000(4)
70	H in H_2O	1.0017(44)	1.0041(3)	1.0034(3)	-0.0007(4)
71	H in H_2O	0.9961(9)	0.9950(3)	0.9955(3)	0.0005(4)
72	H in H_2O	0.9973(9)	0.9977(3)	0.9971(3)	-0.0006(4)
73	H in H_2O	0.9985(10)	0.9958(3)	0.9963(3)	0.0005(4)
74	H in H_2O	0.9988(11)	0.9986(3)	0.9991(3)	0.0005(4)
75	H in H_2O	0.9983(11)	0.9975(3)	0.9977(3)	0.0002(4)
	RMS Error		0.00845	0.00805	
	RMS Continuous / RMS Discrete		0.95322		

Table IV. LEU Benchmark Eigenvalue Results

Case Number	$S(\alpha, \beta)$-treated Isotope	Experiment k_{eff}	Discrete k_{eff}	Continuous k_{eff}	Δk from Discrete
76	H in H_2O	1.0007(16)	1.0012(3)	1.0005(3)	-0.0007(4)
77	H in H_2O	1.0007(16)	1.0013(3)	1.0015(3)	0.0002(4)
78	H in H_2O	1.0007(16)	1.0007(3)	1.0005(3)	-0.0002(4)
79	H in H_2O	1.0006(16)	1.0003(3)	0.9999(3)	-0.0004(4)
80	H in H_2O	1.0007(16)	1.0007(3)	1.0000(3)	-0.0007(4)
81	H in H_2O	1.0007(16)	1.0020(3)	1.0014(3)	-0.0006(4)
82	H in H_2O	1.0038(40)	1.0000(3)	0.9998(3)	-0.0002(4)
83	H in H_2O	1.0024(37)	0.9959(3)	0.9951(3)	-0.0008(4)
	RMS Error		0.00768	0.00846	
	RMS Continuous / RMS Discrete		1.10247		

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Table V. Pu Benchmark Eigenvalue Results

Case Number	$S(\alpha,\beta)$-treated Isotope	Experiment k_{eff}	Discrete k_{eff}	Continuous k_{eff}	Δk from Discrete
97	Graphite	1.0000(20)	0.9993(3)	0.9993(3)	0.0000(4)
98	Be Metal	1.0000(30)	0.9964(3)	0.9962(3)	-0.0002(4)
99	Be Metal	0.9992(15)	0.9975(3)	0.9979(3)	0.0004(4)
100	H in CH_2	1.0000(20)	1.0019(3)	1.0024(3)	0.0005(4)
101	H in H_2O	1.0000(10)	1.0006(3)	1.0001(3)	-0.0005(4)
102	O in BeO / Be in BeO	1.0000(26)	0.9931(3)	0.9922(3)	-0.0009(4)
103	Be Metal	1.0000(26)	1.0021(3)	1.0033(3)	0.0012(4)
105	Graphite	1.0000(110)	1.0116(2)	1.0119(2)	0.0003(3)
106	H in H_2O	1.0024(60)	1.0010(3)	1.0017(3)	0.0007(4)
107	H in H_2O	1.0009(47)	1.0028(3)	1.0024(3)	-0.0004(4)
108	H in H_2O	1.0042(31)	1.0032(3)	1.0026(3)	-0.0006(4)
109	**H in H_2O**	**1.0024(21)**	**1.0079(3)**	**1.0063(3)**	**-0.0016(4)**
110	H in H_2O	1.0038(25)	1.0046(3)	1.0040(3)	-0.0006(4)
111	H in H_2O	1.0029(27)	1.0068(3)	1.0063(3)	-0.0005(4)
112	H in H_2O	1.0000(33)	1.0190(2)	1.0189(2)	-0.0001(4)
113	H in H_2O	1.0000(52)	1.0060(4)	1.0061(4)	0.0001(6)
114	H in H_2O	1.0000(52)	0.9943(4)	0.9939(4)	-0.0004(6)
115	H in H_2O	1.0000(52)	0.9996(4)	1.0002(4)	0.0006(6)
116	H in H_2O	1.0000(32)	1.0043(4)	1.0048(4)	0.0005(6)
117	H in H_2O	1.0000(65)	1.0044(5)	1.0037(5)	-0.0007(7)
118	H in H_2O	1.0000(34)	1.0031(3)	1.0026(3)	-0.0005(4)
119	H in H_2O	1.0000(62)	0.9999(4)	0.9998(4)	-0.0001(6)
	RMS Error		0.02714	0.02726	
	RMS Continuous / RMS Discrete		1.00431		

Table VI. Total RMS Error for 64 Thermal Scattering Comparisons

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

3.3. Detailed Investigation of Case 109, mix-comp-therm-002-case-pnl33

There is very little change in the eigenvalue between the two $S(\alpha,\beta)$ treatments, with the largest change being around 160 pcm for Case 109. This benchmark is a MOX lattice with fuel rods contained in borated water at 1090.4 ppm. Similar benchmarks are tested with the same parameters, but with less boron. A summary of the 6 PNL MOX cases containing boron is given in Table VII.

Table VII. PNL MOX Benchmark Parameters and Results

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		

For the most part, as the amount of boron is decreased in the water, the change in eigenvalue between continuous and discrete S(α,β) treatments for water also decreases. This makes sense since one expects large differences when changing the scattering law for the scattering material (hydrogen in water) as the amount of the scattering material is being reduced in the system. For cases mix-comp-therm-002-case-pnl30 through mix-comp-therm-002-case-pnl35, a definitive trend could not be established relating the eigenvalue differences to the amount of borated water in the benchmark. The MOX lattice benchmark case 106 with 1.7 ppm of boron shows an increase in eigenvalue when a continuous S(α,β) treatment is used whereas all other MOX lattice benchmarks show a decrease.

This case was rerun for both the discrete and continuous treatments using 100,000 source histories per cycle to see the reduction in the standard deviation. The eigenvalues for both cases were 1.0069(1). This further analysis indicates the results do agree with each other within the given uncertainties.

3.4. Detailed Investigation of Case 16, u233-sol-therm-001-case-4

This benchmark case is an unreflected, spherical reactor containing a solution of $U(NO_3)_2$ (uranyl-nitrate) inside an annular shell of Aluminum-1100 with a spherical source. The scattering material of interest for this benchmark problem is hydrogen in water. The five benchmark cases u233-sol-therm-001-case-1 through u233-sol-therm-001-case-5 all contain these same parameters with the concentration of uranyl-nitrate increasing for each case, from 17.14 g/l for case one to 19.82 g/l for case five. There does not appear to be a direct correlation between uranyl-nitrate concentration and the effect on eigenvalue through a different thermal scattering cross section treatment. The eigenvalue differences from the discrete cases appear to fluctuate randomly between the five cases.

This case was rerun for both the discrete and continuous treatments using 100,000 source histories per cycle to see the reduction in the standard deviation. The eigenvalues for both discrete and continuous runs were 1.0009(1), indicating agreement within statistics.

4. CONCLUSIONS

There is a relatively small change in the eigenvalue when comparing discrete and continuous thermal scattering treatments. Of the 64 cases compared, 62 agree at the 95% confidence level, and the 2 cases with differences larger than 3 σ agreed within 1 σ when more neutrons were run in the calculations. The changes in eigenvalue between benchmark cases do not appear to follow a pattern. The changes are small, random, and well within the uncertainty of measured data for reactor criticality experiments. This is to be expected, since the same physical data and basic NJOY processing underlies each treatment.

In reactor criticality experiments, only integrated values of the detailed thermal flux spectrum are of importance and the sharp edges resulting from discrete energy and angle pairs are not observed. In some non-reactor experiments with very few scatters or experiments where the detailed thermal flux spectrum is important, these sharp spikes need to be resolved and this is done through the continuous thermal scattering treatment. Therefore, although the continuous treatment is a more realistic, high-fidelity treatment of thermal scattering, further analyses with experiments consisting of a few scattering events are needed before changing the default MCNP $S(\alpha,\beta)$ data from discrete to continuous.

This work has verified that a change from the traditional discrete treatment to a continuous treatment does not significantly affect the results when analyzing criticality experiments. This conclusion is supported (informally) by a number of ENDF/B-VII.1 evaluators who are using the continuous $S(\alpha,\beta)$ treatment in their data assessments [11]. It is expected that a general release of MCNP6 in 2012 will include both the discrete and continuous $S(\alpha,\beta)$ thermal scattering datasets.

ACKNOWLEDGMENTS

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