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FISSION NEUTRON MULTIPLICITY IN MCNP6 CRITICALITY CALCULATIONS

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ABSTRACT

In the solution of the neutron transport equation, the k-effective eigenvalue is related to the average number of neutrons emitted in fission of the system. However, the fissioning of a nucleus leads to the emission of any number of neutrons with some probability with correlated emission energies that is a function of the incident neutron energy. In general, Monte Carlo codes used for criticality calculations do not use explicit fission multiplicity sampling instead opting for the expected-value outcome approach. As computational methods and resources advance, there is growing interest in high fidelity modeling, including nuclear fission physics modeling. Extensive criticality benchmarks have been established to verify and validate Monte Carlo calculations versus analytic solutions and benchmarked experiments using the expected-value outcome method and no verification-validation work has been done to date on using explicit fission neutron multiplicity models in MCNP6. To determine the effect of sampling fission multiplicity probability distributions during criticality (KCODE) calculations, MCNP6 was modified to allow for the use of neutron fission multiplicity models during criticality calculations along with correlation of neutron emission energies. Previously, MCNP6 did not allow for the use of these models during criticality calculations and only allowed their use in fixed-source problems. It was found that explicit fission multiplicity sampling agreed within two standard deviations of expected-value outcome sampling calculated k-effective values. Various benchmark suites used to test MCNP6 k-effective criticality calculations demonstrated good agreement using explicit fission multiplicity sampling and confirmed the validity of using explicit fission multiplicity sampling in Monte Carlo criticality calculations.

Key Words: **criticality, fission, multiplicity, energy correlation**

1. INTRODUCTION

In the solution of the neutron transport equation, the k-effective eigenvalue is related to the average number of neutrons emitted in fission, $\bar{\nu}$, of the system. It can be shown that if the average number of neutrons emitted in fission and the average neutron energy spectrum is conserved, the criticality of a system remains the same without regard to the actual physical fission process. However, the fissioning of a nuclei leads to the emission of any number of neutrons with some probability that is a function of the incident neutron energy. In addition to the average number of neutrons emitted in fission, the energies of these neutrons have impacts on the neutron spectrum of a system. The fission neutron energy emission spectrum $\chi(E \to E')$ determines the outgoing energy of neutrons and is of importance in the fission process. When multiple neutrons are emitted in a fission event, the correlation of their energies impacts the neutron spectrum. Changes in the neutron spectrum affect the criticality of a system as the energies determine neutron reaction rates in a system.

Historically, Monte Carlo codes have used the expected-value outcome approach to fission neutron production during criticality calculations. Extensive criticality benchmarks have been established to verify and validate Monte Carlo calculations versus analytic solutions and benchmarked experiments using this method [1]. As computational methods and resources advance, there is growing interest in high fidelity modeling. Approximations and methods used due to limited computational resources and missing nuclear data are being replaced with more physical models and data that better reflect the actual physics. These models are being implemented in codes such as MCNP6 to better reflect the underlying physical processes in neutron transport calculations.

2. METHODS OF FISSION EVENT SAMPLING IN MCNP6

There are two distinct but mathematically equivalent methods to sample the number of neutrons emitted in a fission reaction: the expected-value outcome approach and explicit multiplicity distribution sampling. Random sampling introduces variance into the calculated k-effective value. The variance from a certain randomly sampled event can be eliminated by introducing statistical weights effectively replacing the random sampling with the expected value for an event.

2.1. The Expected-Value Outcome Approach

Production level MCNP6 currently uses the expected-value outcome (EVO) approach to determine the number of neutrons emitted in a fission reaction [2]. Consider a neutron collides with a fissile nucleus. The expected number of fission neutrons n emitted due to this collision is given by $n = {}^{\nu\Sigma_f}/_{\Sigma_t}$, where ν is the number of neutrons emitted in fission and Σ_t and Σ_f are the total and fission cross section respectively. To sample the number of neutrons emitted the following algorithm is used: let r = $\nu\Sigma_f/\Sigma_t$

and n $=$ int[r], produce n fission neutrons with probability one and an additional fission neutron with probability r-n. For example, let $\nu\Sigma_f/\Sigma_t$ = 1.75 and sample a random number ξ. If $\xi <$ 0.75, produce two fission neutrons, otherwise produce one fission neutron.

2.2. Explicit Fission Neutron Multiplicity Sampling

Explicit fission multiplicity sampling (EFMS) uses the Lawrence Livermore National Laboratory Fission Library (LLNL Fission Library) [3]. The LLNL Fission Library consists of experimentally obtained probability distributions for the major actinides in addition to the general neutron multiplicity distributions derived by Terrell [4].

In cases where there exist no multiplicity distribution data for a fissioning actinide, MCNP6 uses Terrell's model. Terrell's model assumes fission neutrons will be emitted whenever energetically possible, that the emission of any neutron from any fission fragment reduces the excitation of the fission fragment by ΔE and the total excitation energy from two fission fragments from binary fission has a Gaussian distribution.

The probability of emitting n neutrons in fission is given by

$$P_{n\neq 0} = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{n-1/2}^{n+1/2} \exp\left(\frac{-(x-\bar{\nu}+b)^2}{2\sigma^2} \right) dx.$$

where b is an adjustment factor to preserve $\bar{\nu}$. The probability of emitting zero neutrons uses the same expression with the limits of integration from negative infinity to 1/2.

When experimental data is available for sampling, a table search is done to determine the number of neutrons emitted in fission. When Terrell's model for fission neutrons is employed, the algorithm by Cullen [5] is used to sample the number of neutrons emitted in fission.

2.3. Prompt Fission Neutron Spectrum Differences

MCNP6 uses prompt fission neutron spectra data from the ACE data files for each actinide. The LLNL Fission Library assumes all actinides have the same analytical ENDL Watt spectrum form for fission neutron spectra [6]:

$$W(a, b, E') = Ce^{-aE'} \sinh(\sqrt{bE'}),$$

where $C = \sqrt{\pi \frac{b}{4a}} \frac{e^{\frac{b}{4a}}}{a}$ and E' is the secondary energy neutron. The coefficients a and b vary weakly for each fissile isotope considered. For the case of neutron-induced fission, parameter b is set equal to 1.0 and parameter a is given as a quadratic function of incident neutron energy: $a(E) = a_0 + a_1 E + a_2 E^2$, where the coefficients a_0, a_1, and a_2 are given for 40 isotopes. For multiplicity sampling enabled criticality calculations, the LLNL Fission Library was compiled using the default neutron energy conservation correlation. For a single fission event, neutron energies are sampled independently from the material prompt fission neutron spectrum, and there is no explicit energy conservation.

3. EXPLICIT FISSION MULTIPLICITY SAMPLING VERIFICATION

Explicit fission neutron multiplicity verification was done using k-effective comparisons to the expected-value outcome approach. The VALIDATION CRITICALITY and VALIDATION CRITICALITY EXTENDED benchmark libraries were used for verification. Both test suites [7] are included in all MCNP6 distributions and contain input decks of benchmarked experiments with various major actinides covering fast, intermediate and thermal energy spectra. K-effective values were compared between both fission neutron sampling schemes and the root mean square difference was used to determine an overall measure of agreement for the complete set of benchmarks.

For the purposes of verification, k-effective agreement was defined as an explicit fission multiplicity model k-effective within two standard deviations of the calculated k-effective using the standard approach. In addition, both methods sampled the outgoing fission neutron energies from the ACE data library assuming no correlation between emitted fission neutron energies.

3.1. VALIDATION CRITICALITY Benchmark

Agreement within two standard deviations was found between both sampling methods. Figure 1 shows that in no cases was the difference in k-effective larger than two standard deviations of the expected-value outcome sampling result. The root mean square (RMS) error between the two sampling methods was found to be 0.0380%. Agreement between the average number of neutrons emitted in fission $\bar{\nu}$ was also established to within one percent.

3.2. MCNP6 Extended Criticality Validation Suite Benchmark

Further validation was done using the MCNP6 Extended Criticality Validation Suite. The suite was subdivided into five categories, consisting of a total of 119 input decks with five general types of systems: low enriched uranium (LEU), intermediate enriched uranium (IEU), high enriched uranium (HEU), uranium-233 (U233), and plutonium (PU). The benchmark was run on the Los Alamos National

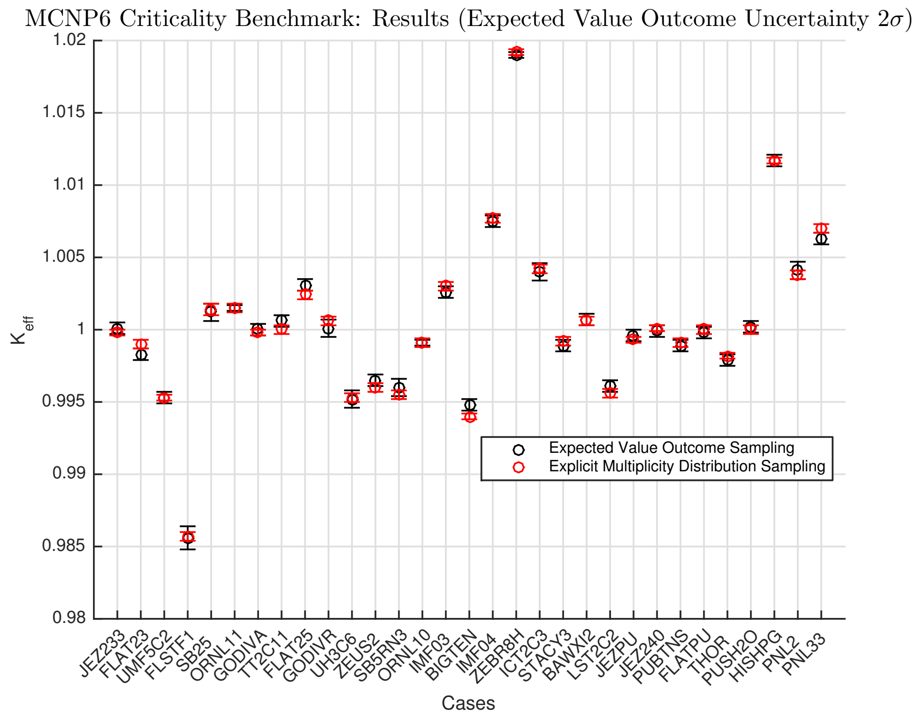


Figure 1: VALIDATION CRITICALITY k-effective Comparison (50000 neutrons per cycle)

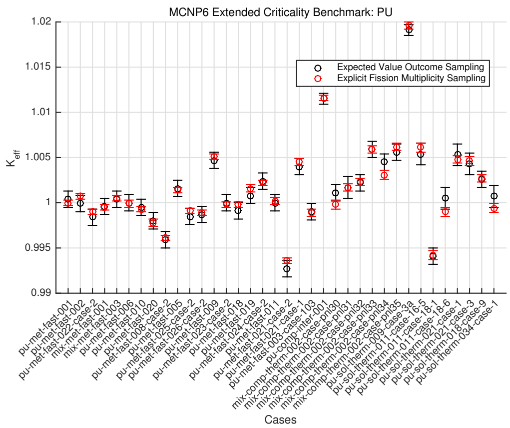
Laboratory cluster Mapache using 10000 neutrons per cycle for 600 cycles, with the first 100 cycles skipped. Overall agreement was found for 91 out of the 119 cases.

Agreement for plutonium cases was found for 27 of 36 cases (Figure 2a). The RMS for the cases was found to be 0.0608%. Cases that were not within two standard deviations of expected-outcome value sampling were a mixture of fast metal systems and thermal solution systems.

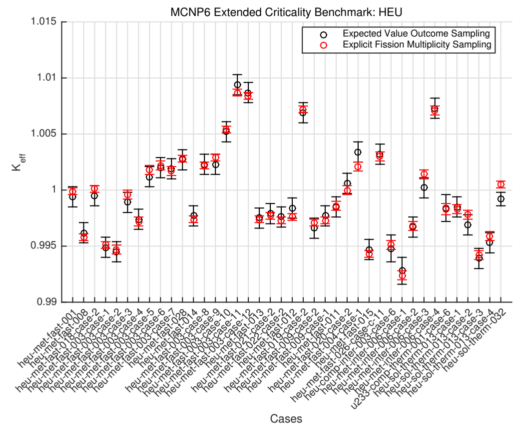
Agreement for high-enrichment uranium systems was found for 33 of 40 cases as seen in Figure 2b. The RMS for the HEU benchmark portion was found to be 0.0529%. Cases that were not within two standard deviations were found to be primarily metal systems in the fast and intermediate neutron energy spectra regions with two thermal solution systems.

Agreement for intermediate-enrichment uranium systems was found for 11 of 17 cases (Figure 2c). The RMS for the IEU benchmark was found to be 0.0587%. Cases that were not found within the two standard deviations were some fast metal and thermal solution systems.

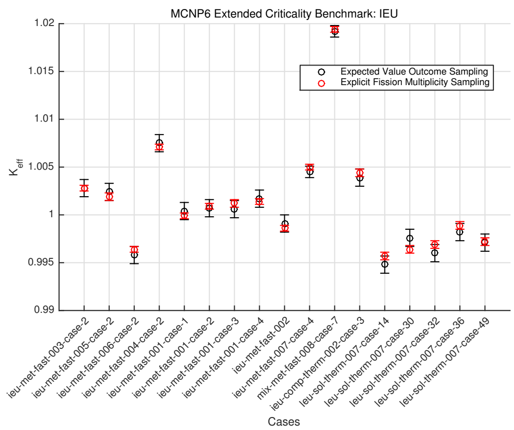
Agreement for low-enrichment uranium systems was found for five of eight cases as seen in Figure 2d. The RMS error was found to be 0.0717% for the IEU benchmark. In this particular case, all three cases found in disagreement were thermal systems. Two cases were liquid solution systems while the other was a mixed composition system.



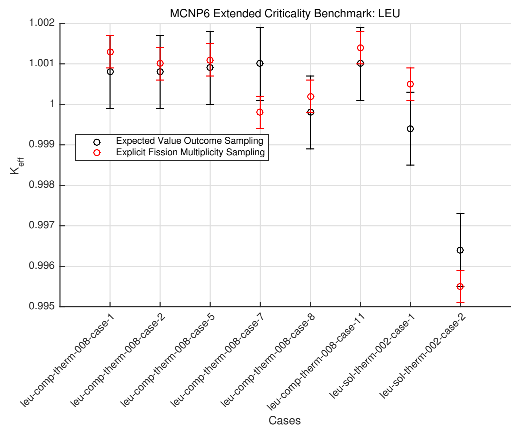
(a) Plutonium k-effective Comparison



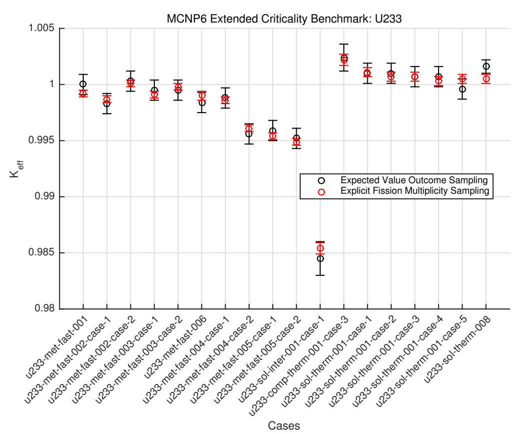
(b) HEU K-effective Comparison



(c) IEU K-effective Comparison



(d) LEU K-effective Comparison



(e) U233 K-effective Comparison

Figure 2: Extended Criticality Validation Suite Results

Agreement for uranium-233 systems was found for 15 of 18 cases. The RMS error was determined to be 0.0538% for uranium-233 systems. The three cases that were found to be in disagreement were one fast metal system and two thermal solution systems (Figure 2e).

Good agreement was found for expected-value outcome and explicit fission multiplicity sampling with ACE (ENDF) fission neutron spectra data. Some differences exist but are found to be at most three standard deviations from the calculated expected-value outcome k-effective. Explicit fission multiplicity sampling k-effective and $\bar{\nu}$ agrees well with default expected-value outcome sampling.

4. EXPLICIT FISSION MULTIPLICITY SAMPLING WITH LLNL FISSION LIBRARY NEUTRON ENERGY SPECTRA SAMPLING

The option exists to allow sampling of emitted fission neutron energies from the LLNL Fission Library. K-effective comparisons were made between the expected-value outcome sampling and fission multiplicity and neutron fission energy sampling approaches. Agreement was found for only 19 of 119 cases. Testing of LLNL Fission Library prompt neutron fission spectra was done to determine the impact of using another set of data in criticality calculations. The differences in the ENDL and ACE fission neutron energy spectra caused substantial differences in calculated k-effective values.

4.1. VALIDATION CRITICALITY Benchmark

K-effective results for explicit fission multiplicity sampling with ACE and ENDL fission neutron energy spectra were compared as seen in Figure 3. The root-mean-square deviation was found to be 0.0691%.

4.2. MCNP6 Extended Criticality Validation Suite Benchmark

One case of 36 was found to be in agreement as seen in Table 4a for plutonium systems. Plutonium isotopes' fission neutron energy spectra are given by a Simple Maxwellian distribution in ENDF data evaluations as described earlier. ENDL fission spectra for plutonium isotopes are given by a Watt spectrum. No agreement was expected and k-effective comparisons support this conclusion. The RMS error was found to be 0.6759%.

Eleven of 40 cases were found to be in agreement for HEU systems as seen in Table 4b. Similar to plutonium, some uranium isotopes' fission neutron energy spectra are represented by a Simple Maxwellian distribution. The RMS error was found to be 0.4304%. Thermal systems show the greatest differences in k-effective, suggesting changes in k-effective are due to changes in the average energy of a neutron causing fission in the system.

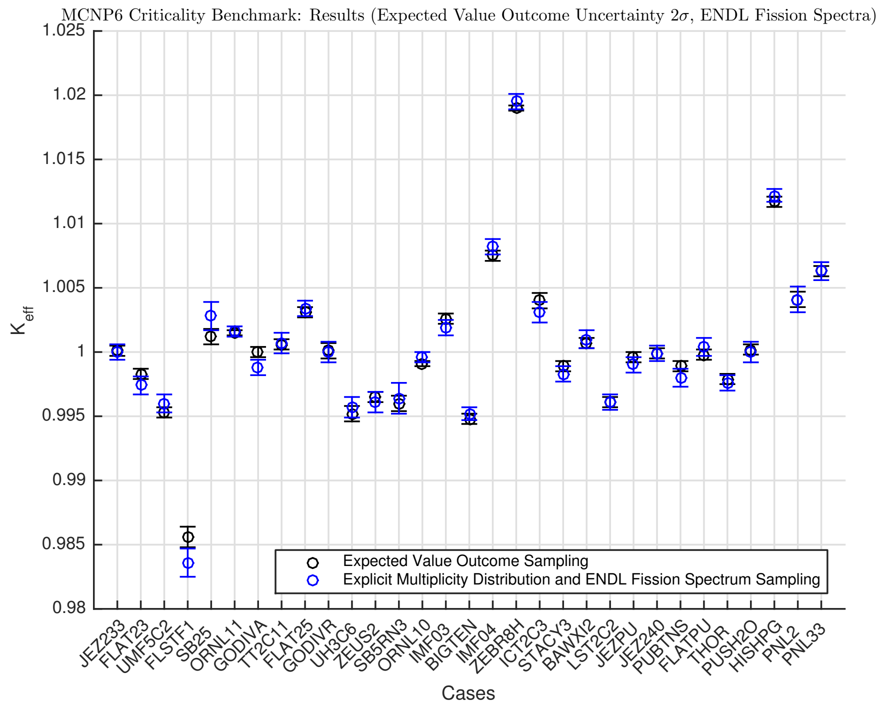


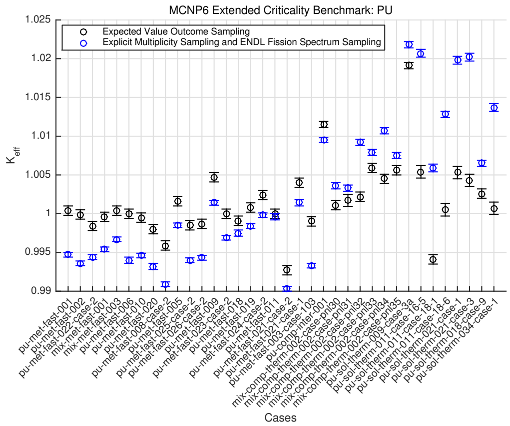
Figure 3: VALIDATION CRITICALITY Chi Sampling k-effective Comparison (50000 neutrons per cycle)

No cases of 17 were found to be in agreement for IEU systems. k-effectives were found to disagree by three standard deviations in almost all cases as can be seen in Table 4c. In all thermal spectrum cases, the k-effective of explicit multiplicity and ENDL spectra sampling was found to be greater than the expected-value outcome k-effective. The RMS error was calculated as 0.6852%.

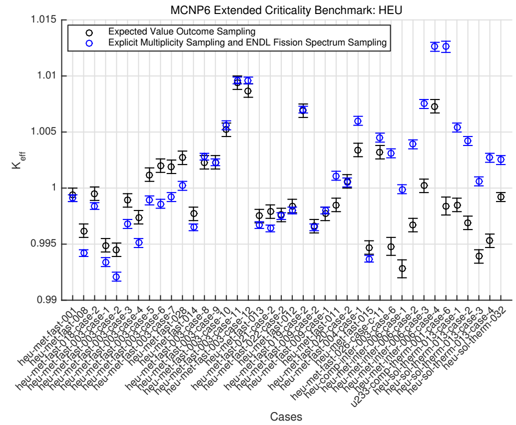
Two of eight cases were found to be in agreement for LEU systems. Thermal solution systems showed the most disagreement as seen in Figure 4d. The RMS error was found to be 0.2763%. Thermal solution k-effective differences imply differences in the thermal fission cross section for uranium isotopes due to differences in the ENDF and ENDL evaluations as expected.

Six of 18 uranium-233 systems were found to be in agreement. In particular, fast metal uranium systems agreed relatively well as seen in Figure 4e. However, thermal solution uranium-233 systems were found to be in substantial disagreement (3σ). The sole intermediate neutron spectrum case was found to differ by Δk of approximately 0.02. The RMS error was found to be 0.8797%, primarily driven by differences in k-effective of thermal spectra, solution-based, uranium-233 systems.

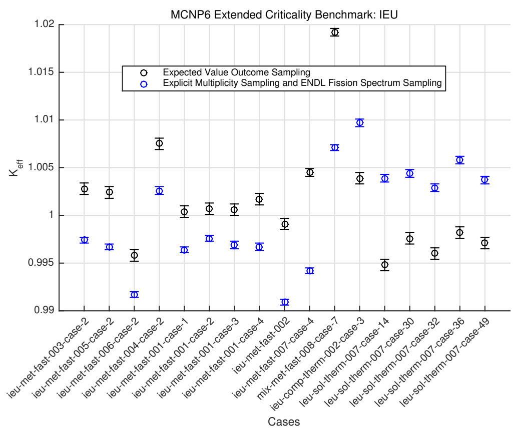
Expected-value outcome and explicit fission multiplicity sampling k-effectives using both the ENDF and ENDL neutron fission spectra showed substantial disagreements. This was expected due to the differences in models used for major actinides in the benchmarks. For cases where ENDF and ENDL fission neutron energy spectra were similar showed improved agreement.



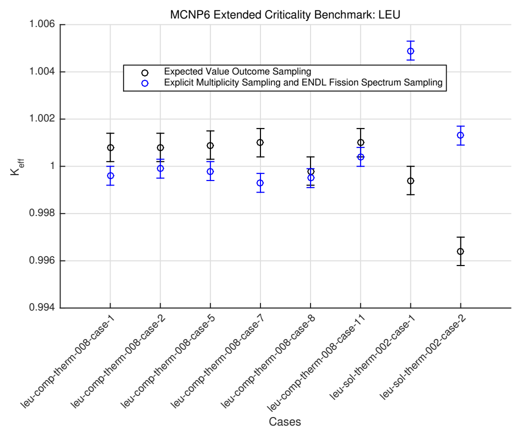
(a) Plutonium k-effective Comparison



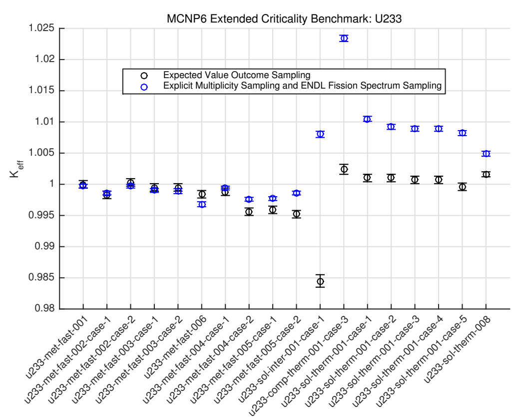
(b) HEU K-effective Comparison



(c) IEU K-effective Comparison



(d) LEU K-effective Comparison



(e) U233 K-effective Comparison

Figure 4: Extended Criticality Validation Suite Results-ENDL Neutron Spectra Sampling

5. CONCLUSION

This work focused on the sampling methods used in MCNP6 criticality calculations. With advances in computation methods and resources, the increasing interest in high fidelity modeling of nuclear systems makes it necessary to implement physical models and data that accurately reflect the underlying physics. For nuclear fission, explicit fission multiplicity data exists for various important actinides. Using the Lawrence Livermore National Laboratory Fission Library, this data was implemented into MCNP6, and MCNP6 was allowed to use explicit fission multiplicity sampling for criticality calculations. Previously no work had been done on explicit fission multiplicity. It was found that explicit multiplicity sampling matched expected-value outcome sampling for most cases within two standard deviations. Explicit fission multiplicity sampling with neutron energy spectra sampling shows disagreement due to differences in neutron energy spectra evaluation differences between ACE and ENDL. Preliminary study of correlated fission neutron energies showed systematic differences in k-effective. Using simple correlation schemes, differences in k-effective are highly suggestive of not well understood impacts of energy correlation in k-effective calculations. Future work will focus on quantifying the impact through analysis of the neutron transport equation with correlation fission neutron energies.

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