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Deleterious Feedback From Equilibrium Xenon and Bias in 3D Power Distribution When Insufficient Neutron Histories Per Cycle are Used in Monte Carlo Simulation of CANDU6

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1. Introduction

Full-core Monte Carlo (MC) criticality simulation is becoming a tractable problem with the availability of many MC codes developed worldwide specifically for full-core analyses coupled with computing hardware advances and cost reductions. Reliable local tallies (e.g., flux and power) in heterogeneous reactor lattices should be the targets of these simulations with potential applications in design calculations and regulatory compliance. However, the MC analyst must selective appropriate MC simulation parameters—number of inactive cycles, number of active cycles, and number of neutron histories per cycle (*N*)—to obtain reliable results. The number of inactive cycles is usually chosen through a subjective procedure of visual inspection of Shannon entropy and Center of Mass (CoM) plots. These metrics encode the evolution of the spatial distribution of and density of fission sites as function of cycle number, and asymptotic values are obtained during the inactive cycles during which the fission source converges to the fundamental mode (FM) from the initial source guess and the higher-order modes decay away. Tallies are accumulated during active cycles, the number of which is free to be chosen by the analyst to obtain an acceptable statistical uncertainty level of the tallies. The *N* is the most important parameter, and if an insufficient *N* is chosen, physical-numerical oscillation of the fission source and flux distribution about the mode obtained during inactive cycles occurs, and the obtained 3D power tallies exhibit power tilts. The tally variances should be proportional to the inverse of the total number of simulated particles N_{tot} (# active cycles times *N*).

Determining the optimal *N* (and number of inactive cycles) is a nontrivial task and can consume significantly more computational resources and analysis man-hours than the targeted application of the full-core MC model. Here "optimal" is defined as the minimum *N* that guarantees suppression of the numerical power tilts such that local power tallies are unbiased estimates of the 3D power distribution and FM. In benchmarking studies to provide a "reference solution", *N* is usually set to some arbitrarily large value, but this approach is not feasible for design and regulatory calculations due to the high cost of total number of neutrons simulated in inactive cycles. Complicated methodologies [1] to predict the optimal *N* require other parameters of the reactor of interest (dominance ratio, bias estimates of initial fission source distribution, etc.) that are not known a priori and require preliminary analysis and/or capabilities that are not implemented in all MC codes or only available in development versions. Furthermore, examples of the optimal *N* for the different reactor classes—fast versus thermal spectrum, tight pitch light water lattice versus heavy water or graphite moderated with widely spaced fuel channels, etc.—are not reported in literature. Values of the MC simulation parameters used in full-core analyses are usually just reported but with limited or no justification of how or why those parameters were selected. Reference [2] suggests more work is needed for determining neutrons/cycle (i.e., *N*) specifically for large reactors and very loosely coupled problems for providing sufficient counts in mesh bins for reliable distribution-based statistical tests.

The reference reactor design and full-core MC model for the present study is a 1/8th symmetric, CANDU6 lattice fueled with an equilibrium-burnup 37-element fuel bundle previously described in [3,4,5,6]. For full-core MC analysis of CANDU reactors, representative of pressure tube type–heavy water reactors, a wide range of MC simulation parameters have been used. A study using the McCARD MC code simulated a full-core CANDU6 model for few-group constant generation including local lattice cells with reactivity devices using 1200 cycles (200 inactive and 1000 active cycles) with 1 million *N* [7]. Another full-core CANDU6 study [8] proposed a new "enhanced batch method" using 50 inactive plus 200 active cycles per batch with 1 million *N*. A single MC simulation using the MCNP code to obtain bundle and channel power tallies uses 10 batches. The study goal was to obtain improved estimation of the real local power uncertainties and did not directly address the power tilt phenomena observed in full-core CANDU simulations. However, the authors strongly recommended in the conclusions that more neutrons per generation (or cycle) and more tally batches be simulated to obtain more reliable tally means. A subsequent study [9] also using a MCNP full-core CANDU model with local power tallies referenced the simulation procedure of Ref. [8], but used the "brute-force method" (we call this the Central Limit Theorem (CLT) approach) where multiple independent MC runs are performed using different random number seeds and aggregated tally results are obtained from the sample statistics. Thirty-two independent simulations using 200 inactive cycles and 1000 active cycles but only 10,000 *N* were used in Ref. [9].

A second issue that has been largely unaddressed by the MC community is the proper of selection of *N* and the other simulation parameters in the fission-source convergence context in the presence of multi-physics feedback. ^{135}Xe is one of the most important fission products in thermal reactor analysis because it has the largest thermal energy absorption cross-section of any known isotope (2.6 million b). Radioactive ^{135}Xe (9.1 h half-life) is produced by direct-fission yield and through decay of the parent ^{235}I (6.57 h half-life). CANDU reactors and other natural-uranium-fueled power reactors operate with high thermal fluxes, and approximately 90% of ^{135}Xe is consumed by neutron capture, so xenon has a large effect on reactivity and spatial power distribution in large, spatially decoupled CANDU cores. Most production MC codes used for reactor analysis including MCS [10], the code used in the present study, implement "equilibrium xenon" algorithms to iteratively update the ^{135}Xe/^{135}I concentrations and other important saturating fission products during the active cycles based on the tallied reaction rates and flux during the cycles [11], [12], [13], [14], [15]. Figure 1 shows the relative difference in the CANDU6 bundle powers from reference MC CANDU6 simulations with and without equilibrium xenon. Xenon flattens the power distribution by decreasing the power of the high power bundles (usually in central core regions) and increasing the power of the lower power bundles. The changes in local bundle powers, serving as a surrogate for the 3D power distribution, are on the order of a percent, so a full-core MC simulation of a CANDU reactor aiming to obtain accurate local power tallies, must consider xenon. The radial power distributions within fuel bundles are also affected by xenon through a spatial-self-shielding effect with the ring 4 (outer) fuel elements power higher by a few percent and inner-ring fuel element powers suppressed.

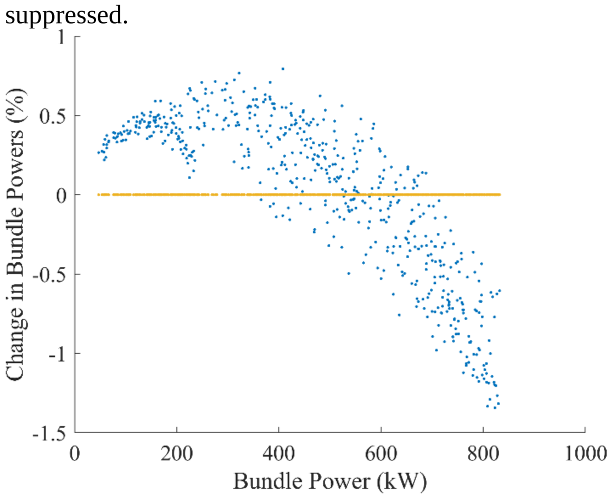

Fig. 1. Change in CANDU6 bundle powers relative to a xenon free core from saturated xenon distribution at full power simulated using the equilibrium xenon option in MCS.

The previous study [4] established through Shannon entropy analysis between 5 million and 10 million neutrons per cycle as the optimal *N* for the 1/8th symmetric CANDU6 model with modified adjuster rod design [4], and 120 inactive cycles are needed for source convergence from a uniform initial source distribution. Shannon entropy plots for select equilibrium xenon cases are shown in Fig. 2. Further investigation of the power tilt phenomena using 100 independent 250,000 *N* simulations in Refs. [4,5] showed for the xenon-free core, the power tilts appeared to be random fluctuations about the reference power distribution established from a 10 million *N* simulation. However, the CLT study [5] repeated for the equilibrium-xenon core showed small but non-negligible autocorrelation of the bundle power relative errors with the average bundle powers of the 250,000 *N* runs in high bundle power positions systematically underestimating the 10 million *N* reference solution and slight overestimation of bundle powers in low power positions at the core periphery. The initial theory proposed in [5] was that 10 million *N* might be insufficient when simulating equilibrium xenon and a small power tilt could be contaminating the reference power distribution.

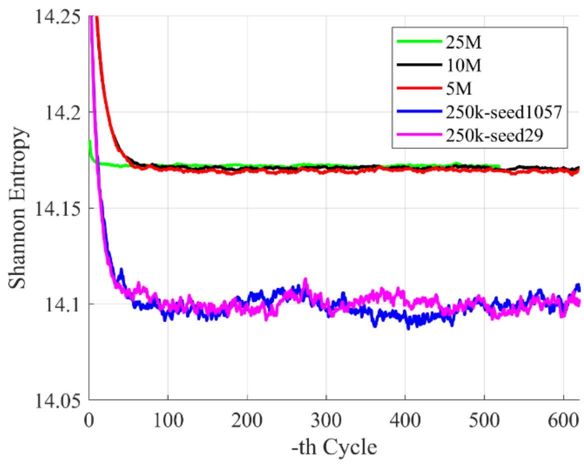

Fig. 2. Shannon entropy plots for equilibrium-xenon simulations. Low *N* entropies fluctuate around lower asymptotic values indicating presence of power tilts while curves overlap for *N* greater than 5 million suggesting these power distributions are unbiased estimates of the true FM.

This study investigates further the power tilts, source convergence, and optimal *N* issues for the equilibrium-xenon CANDU6 MC simulation. The key finding is when insufficient *N* is used, the power tilts are random fluctuations about a power distribution that is not the true fundamental mode. Batch methods or CLT approaches cannot be used in full-core MC analyses when multi-physics feedbacks such as equilibrium xenon are present, and determining the optimal *N* is essential to obtain reliable results. In section 2, 10 million *N* is established as being in fact sufficient for the 1/8th symmetric CANDU6 model with equilibrium xenon through cross validation of the original reference solution from [5] with additional independent reference simulations. The severity of the bias in power distribution as function of *N* is investigated in section 3 by additional CLT studies of xenon-free and equilibrium-xenon simulations using 10,000 *N*.

2. Optimal *N* for equilibrium xenon CANDU6

2.1. CLT methodology

The Gaussian property of sample means is an asymptotic property of the CLT as the sample size becomes large. The CLT has no formally stated sample size restrictions or requirements, but generally a twenty to thirty simulations would be the minimum required. The study in Ref. [9] used 32 independent simulations. Increasing sample size if allowed by available resources is always preferred and more robust statistical arguments can be made from the derived confidence intervals. We recommend at least a sample size of 100 simulations be used when practical.

After simulating M independent simulations initialized with different random number seeds and using the same number of inactive and active cycles and *N*, the average bundle power is calculated as

$$\bar{P}_b = \frac{\sum_{i=1}^{M} P_{b,i}}{M}, \qquad (1)$$

where $P_{b,i}$ is the bundle power from the i^{th} simulation. An average bundle power calculated from Eq. (1) should be an unbiased estimator of the true bundle power. The sample standard deviation for the bundle power is

$$\sigma_b = \sqrt{\frac{\sum_{i=1}^{M}\left(P_{b,i}-\bar{P}_b\right)^2}{M-1}}. \qquad (2)$$

Physically, Eq. (2) quantifies the magnitude of the variation in bundle power at that position from simulation to simulation from the power tilt phenomenon and the baseline stochastic variations in element and bundle powers inherent to the Monte Carlo calculation.

For hypothesis testing and confidence interval analysis when comparing bundle power estimates, the CLT gives the standard deviation of the sample mean as the appropriate metric

$$\sigma_{CLT} = \frac{\sigma_b}{\sqrt{M}} = \sqrt{\frac{\sum_{i=1}^{M}\left(P_{b,i}-\bar{P}_b\right)^2}{M(M-1)}}. \qquad (3)$$

Under the Gaussian assumption of the CLT, the true mean is expected to lie within the interval $\bar{P}_b \pm 2\sigma_{CLT}$ at β = ~95% confidence. If the procedure is repeated many times producing Z unique samples of M simulations in each sample, a dataset of average bundle powers $\bar{P}_{b,j}$ with j = 1,2,...,Z is obtained. Plotting $\bar{P}_{b,j}$ in a frequency plot will yield a histogram that closely resembles a Gaussian distribution and the mean of all $\bar{P}_{b,j}$ will be an excellent estimate of the true mean. Obtaining *Z* samples each with at least 100 full-core MC criticality simulations of the CANDU to make direct inference about the true bundle power mean is not practical. However, plotting $\sigma_{CLT,j}$ in a frequency plot will also yield a histogram resembling a Gaussian distribution with a mean very close to the sample standard deviation of $\bar{P}_{b,j}$; any $\sigma_{CLT,j}$ is an unbiased estimator of the expected standard deviation of $\bar{P}_{b,j}$ using fixed simulation number *M* in a sample. These relationships allow the CLT to be used establish intervals $\bar{P}_b \pm \alpha\sigma_{CLT}$ within which the true mean is expected lie at β confidence levels.

2.2. Comparison of equilibrium xenon reference runs

To check for a minor power tilt contaminating the 10 million *N* reference solution for the equilibrium-xenon core, two additional 10 million *N* simulations initialized with different random number seeds are simulated and compared with the CLT dataset of 100 independent simulations using 250,000 *N* from Ref. [5]. Figure 3 shows the bundle relative errors to the seed 2 case power distribution. The average bundle powers from low *N* simulations exhibit nearly identical error autocorrelation with high bundle powers systematically underestimated. The seed 3 results are also nearly identical. From these results, we conclude 10 million *N* is sufficient to for the equilibrium-xenon core, and the source of the error autocorrelation is from the low *N* simulation data.

To confirm this conclusion, a 25 million *N* reference simulation is performed. The 10 million *N* seed 1 bundle powers are compared to this result in Fig. 4. The near perfect agreement in the power distributions confirm that 10 million *N* with equilibrium xenon multi-physics on is an acceptable number of histories per cycle to fully suppress the power tilts in the 1/8th CANDU6 model.

3. Investigation of bias in low *N* power distributions

Figure 5 reproduces the xenon-free results from [5] for 100 independent 250,000 *N* simulations. The results of a new CLT study of 100 xenon-free simulations using reduced *N* to 10,000 neutrons per cycle and 120 inactive cycles and 500 active cycles are shown in Fig. 6. The magnitude of the power tilts is larger for the very low *N* cases so the magnitude of the scatter of the CLT bundle powers and standard deviations of the means are larger than the 250k *N* results. The relative errors are also well-distributed with random sign of the errors with acceptable coverage by the confidence intervals. For xenon-free case, the CLT approach appears to be an alternative method to obtain power distribution estimates at less computational cost than an optimal reference solution and does not require knowledge of the optimal *N*, which itself is expensive to determine from computational costs and man-hours spent on analysis.

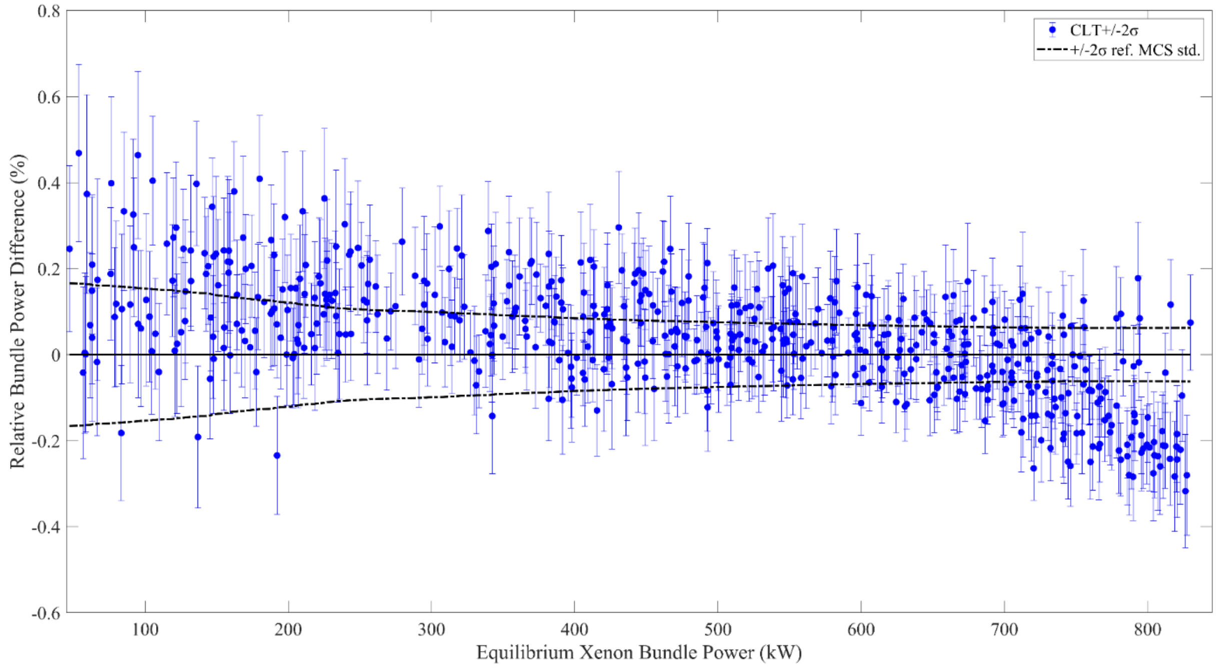

Fig. 3. Comparison of CLT bundle power estimates from 100 independent 250,000 *N* simulations to the equilibrium xenon reference solution (seed 2) showing multi-physics feedback induces bias in power distribution relative to the fundamental mode when insufficient *N* is used. All 250k *N* used 120 inactive cycles and 500 active cycles.

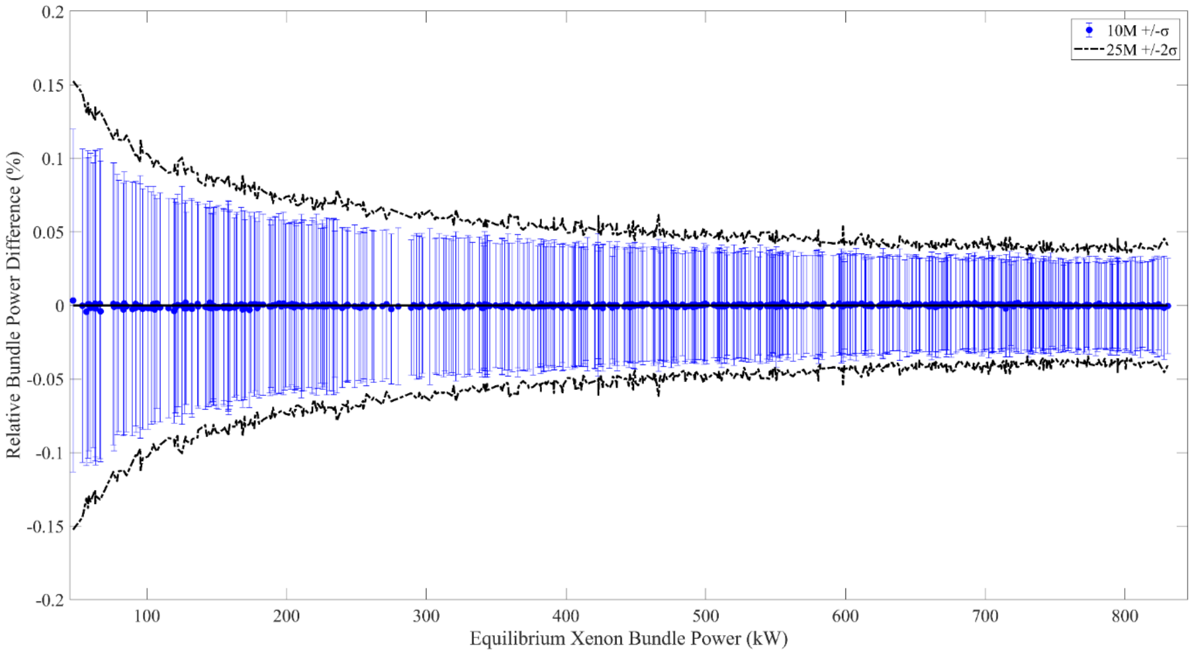

Fig. 4. Comparison of the bundle powers from 10 million *N* simulation (seed 1) to the 25 million *N* results. All of the bundle powers relative errors are less than 0.01%, so the 10 million *N* power distribution is reliable estimate of the FM.

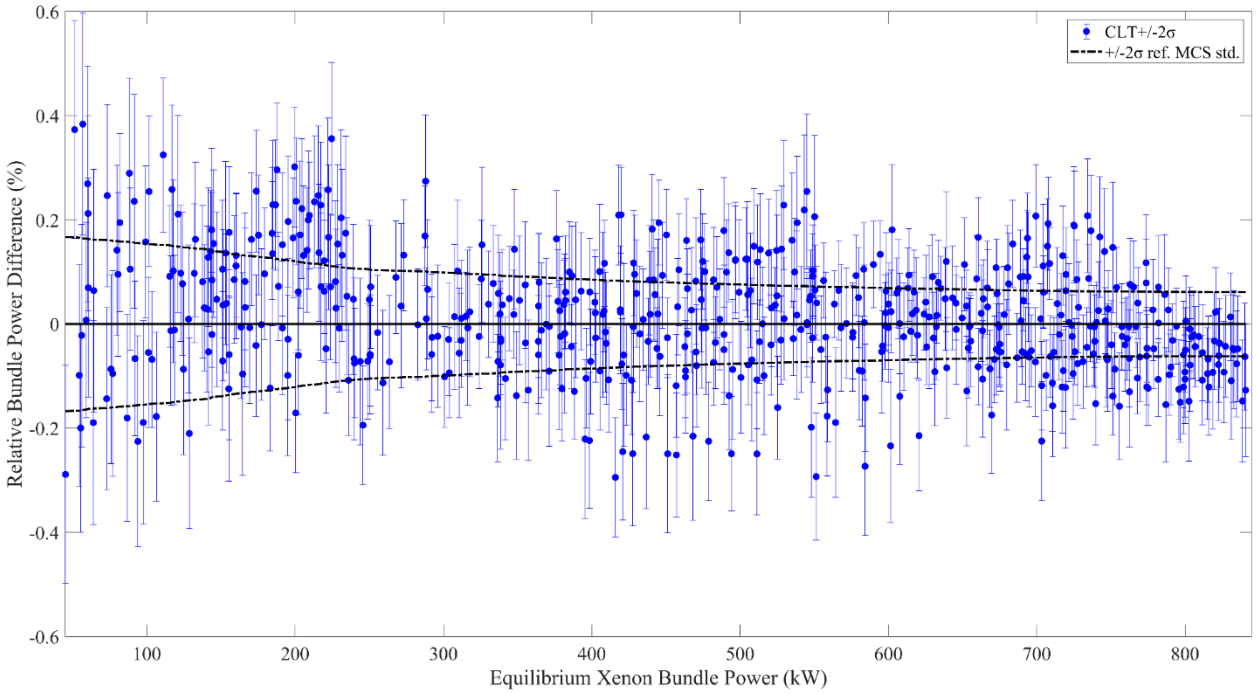

Fig. 5. Comparison of CLT bundle power estimates from 100 independent 250,000 *N* simulations to the xenon-free reference solution showing randomly distributed bundle power errors and acceptable coverage of mean values by confidence intervals.

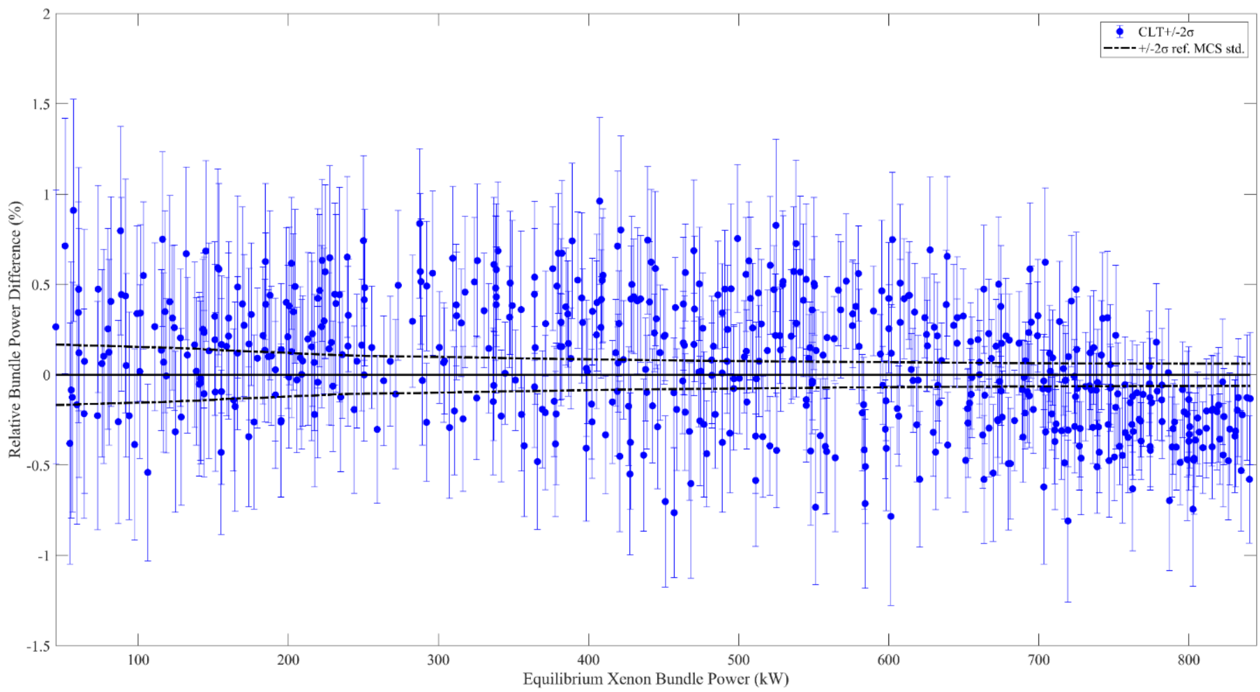

Fig. 6. Comparison of CLT bundle power estimates from 100 independent 10,000 *N* simulations to the xenon-free reference solution showing randomly distributed bundle power errors and acceptable coverage of mean values by confidence intervals.

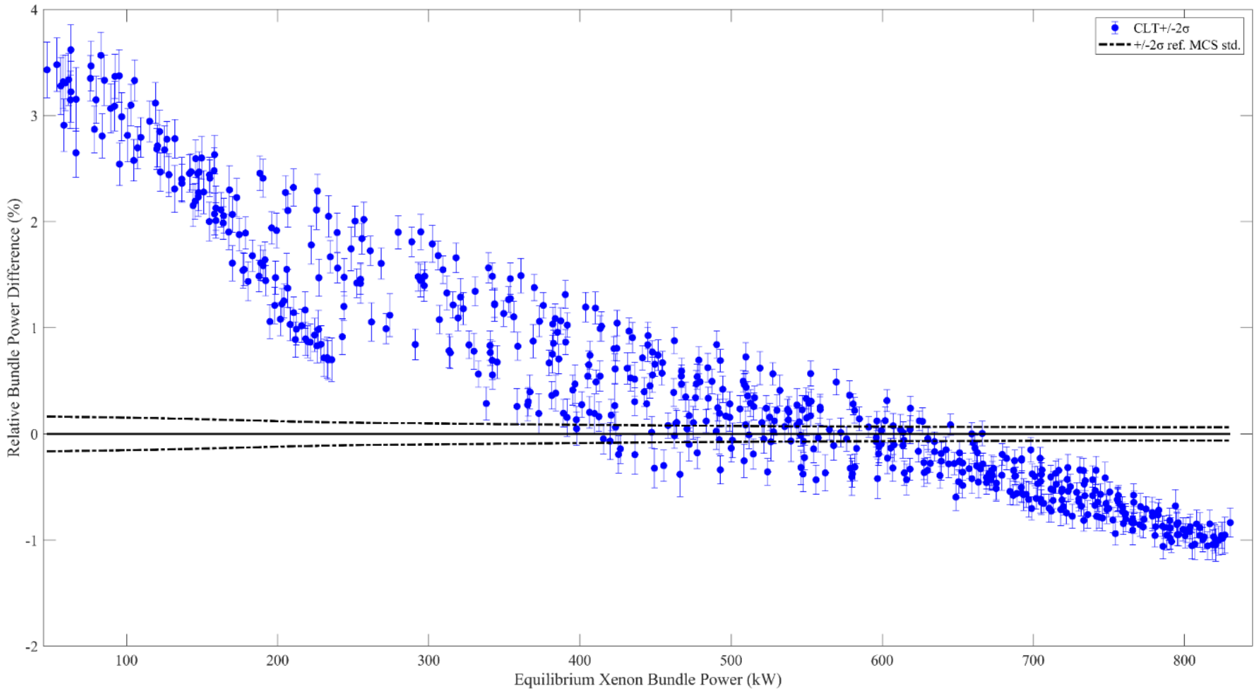

Fig. 7. Comparison of CLT bundle power estimates from 600 independent 10,000 *N* simulations to the equilibrium-xenon reference solution showing multi-physics feedback induces bias in power distribution relative to the fundamental mode when insufficient *N* is used. All 10,000 *N* used 120 inactive cycles and 500 active cycles.

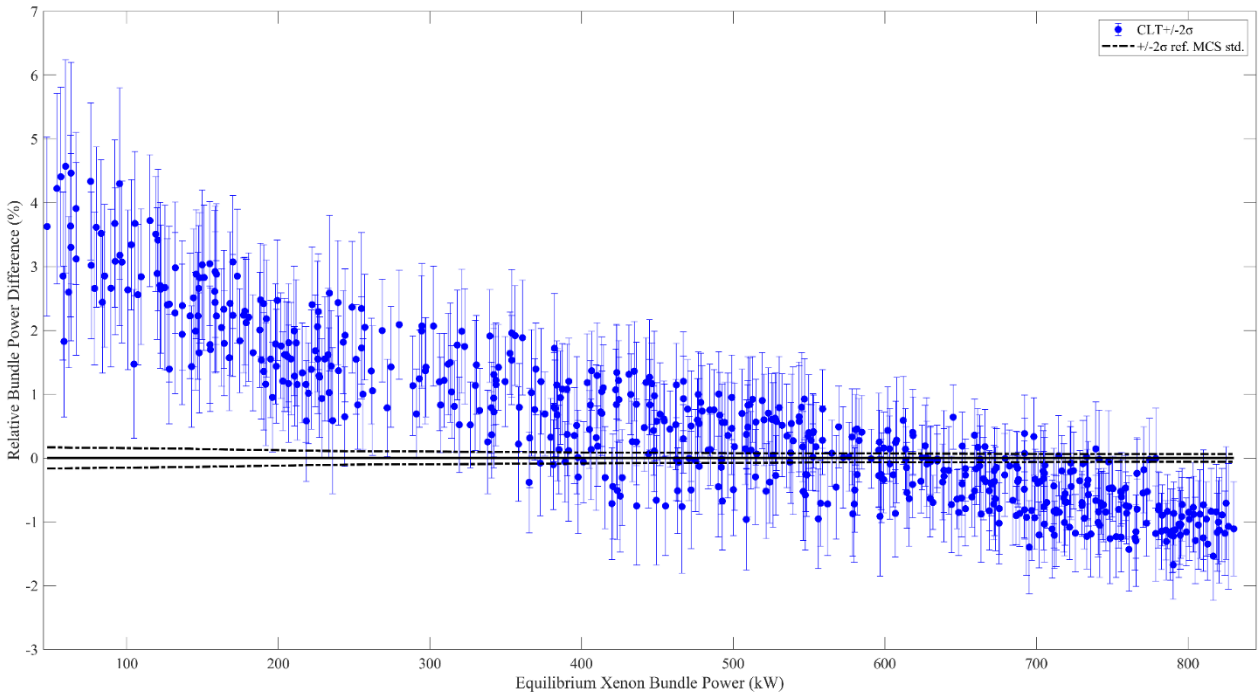

Fig. 8. Comparison of CLT bundle power estimates from 100 independent 10,000 *N* simulations to equilibrium-xenon reference solution showing multi-physics feedback induces bias in power distribution relative to the true fundamental mode when insufficient *N* is used. The 10,000 *N* simulations used 500 active cycles but number of inactive cycles was increased and randomized between 750 and 1000 cycles confirming the bundle power bias is attributable to the equilibrium xenon calculation and insufficient *N* condition and not from insufficient number of inactive cycles.

To comprehensively investigate the influence of the multi-physics coupling on power distribution, an additional set of 600 simulations using 10,000 N with equilibrium xenon were generated. The larger dataset suppresses the magnitude of random scatter arising from simulation-to-simulation power tilts making visual interpretation of confidence intervals straight forward. Figure 7 shows systematic bias in the low N power distribution with suppression of power in the high-power bundles and overestimation of the low-power bundle powers. This strong flattening effect changing bundle powers by several percent is in addition to the change in bundle powers from the true equilibrium xenon distribution shown in Fig. 1. The power distribution bias far exceeds the CLT-derived confidence intervals.

An initial peer review of the significant results in Fig. 7 suggested 120 inactive cycles might be insufficient to guarantee fission source convergence and higher order modes could be contaminating the results. The CLT study was repeated with an additional 100 simulations using 10,000 N but the number of inactive cycles was randomly sampled between 750 and 1000 cycles for each simulation. The period of the Shannon entropy oscillations in Fig. 2 appears to be approximately 100 cycles so by randomly sampling over a range of 250 cycles the initial fission source distribution when active cycles begin are further randomized. Figure 8 compares the CLT bundle powers to the reference solution. The same strong flattened power distribution observed in Fig. 7 is present strongly suggesting an equilibrium xenon effect coupled with the power tilts when insufficient N is used corrupts the Monte Carlo criticality simulation. From these empirical results, the batch method or CLT approach cannot be used with low N when multi-physics coupling is activated.

4. Preliminary assessment of real-to-apparent variance for CANDU local power tallies

In MC criticality simulation, generation or cycle tallies are not independent because fission sites from the preceding cycle are used as the fission source in the current cycle, as well as renormalization of cycle neutron number or neutron weights to preserve N. The tallies accumulated during the active cycle are correlated to the tallies in previous cycles referred to as “inter-cycle correlation”. The quoted statistical uncertainty for a tally result from a single MC simulation is the “apparent” variance and this variance can underestimate the real variance of the underlying radiation transport process due to the inter-cycle correlation. Sample standard deviations calculated from Eq. (2) using the CLT datasets provides “real” variance estimates for the CANDU local power tallies because the simulations are independent. Real-to-apparent variance ratios have been calculated confirming the underestimation, but most studies have been limited to local (pin) or assembly powers in PWR lattices [16,17]. There are nontrivial differences in the neutron transport process (migration and diffusion lengths) and in the strength of the spatial-generational correlations of fission sites between heavy water lattices and light water lattices (as well as other reactor types such as fast reactors), so the MC community should quantify the real-to-apparent ratios of local tallies for all reactors under study and determine how much of underestimation is a numerical aspect of the power-iteration method of MC criticality simulation and how much is lattice specific or neutron transport related.

Figure 9 compares the bundle power sample standard deviations for all bundle positions from all simulations. The N_{tot} was not preserved for the different N cases, so no strong claims can be made about the relationship between σ_b and N. For a given N, low power bundles tend to have higher uncertainties as well as increasing simulation-to-simulation variation in the high-power bundles. Closer examination of the 250,000 N data in Fig. 10 shows close agreement σ_b for xenon-free and equilibrium-xenon cases expect for the divergence in the high power bundles with the equilibrium xenon uncertainty increasing at a higher rate. Closer examination of the 10,000 N data in Fig. 11 shows close agreement between the cases but here the much larger magnitude of the power tilts might be masking differences between the xenon-free and equilibrium-xenon calculations. For completeness, Fig. 12 shows σ_b in absolute terms (kW units) as function of bundle power. The positive trend means higher power bundles have higher absolute uncertainties but relative error is smaller.

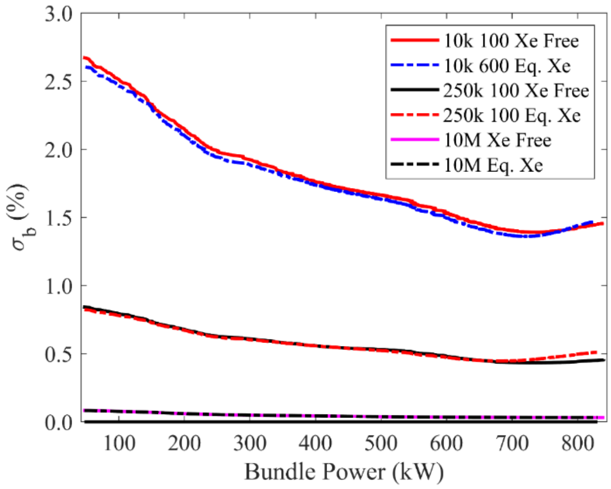

Fig. 9. Bundle power relative sample standard deviations from equilibrium-xenon and xenon-free simulations.

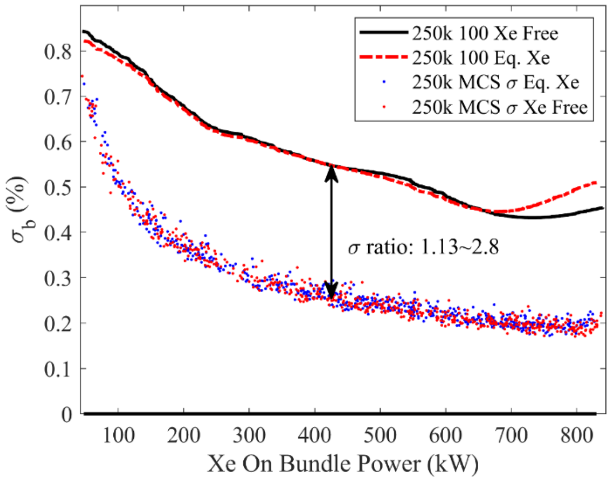

Fig. 10. Bundle power relative sample standard deviations from equilibrium-xenon and xenon-free simulations using 250,000 *N* compared with apparent standard deviation from single MCS simulation.

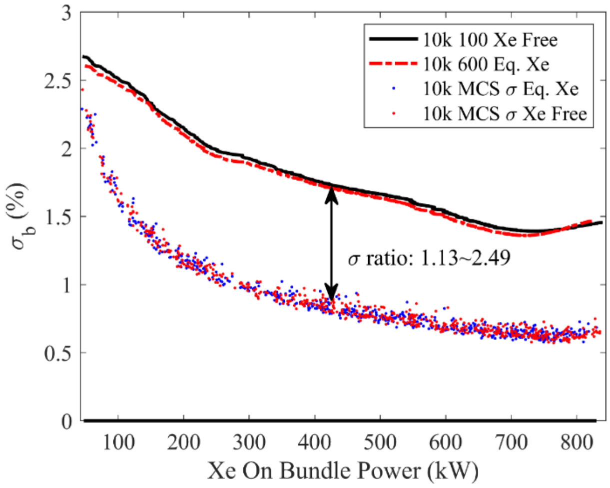

Fig. 11. Bundle power relative sample standard deviations from equilibrium-xenon and xenon-free simulations using 10,000 *N* compared with apparent standard deviation from single MCS simulation.

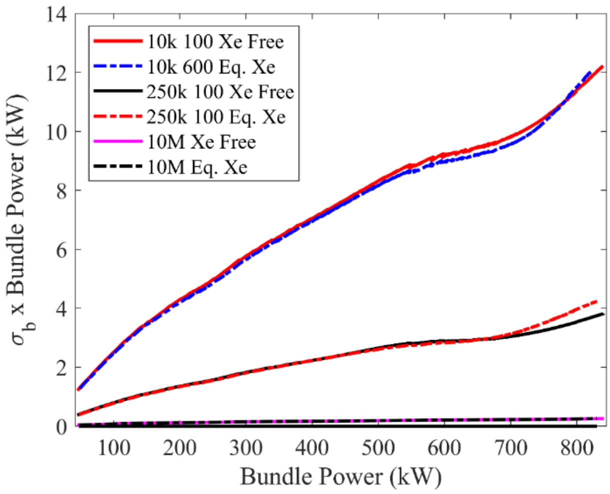

Fig. 12. Bundle power absolute standard deviations from equilibrium-xenon and xenon-free simulations.

Figures 10 and 11 also show apparent standard deviations for the bundle powers from a single MCS simulation drawn at random from the CLT datasets. For 250,000 *N* case (Fig. 10), the standard deviation ratio (the ratio between real standard deviation estimate from the sample standard deviation and MCS-calculated apparent standard deviation) is in 1.13 - 2.8 range. Also, the ratio for 10,000 *N* case values (Fig. 11) is in the 1.13 - 2.49 range. Underestimation of the real variance is usually attributed to the inter-cycle correlation. However, the apparent standard deviations from a single low *N* simulation does not encode all the variance information from power tilts, so this underestimation observed here likely has contributions from both inter-cycle correlation and the power tilt phenomenon. A CLT study using 10 million *N* simulations (with negligible power tilts) is ongoing to isolate the inter-cycle correlation effect on the real-to-apparent standard deviation ratio for local power tallies in the CANDU lattice.

4. Discussion

The results from the present study indicate the power tilts present in full-core Monte Carlo CANDU simulations arising from the use of insufficient *N* are the same magnitude as real physical phenomena such as the xenon effect on the power distribution. Using insufficient *N* with multi-physics coupling (equilibrium xenon) to the power-iteration method of MC criticality simulation induces bias in the converged fission source and power distributions with stochastic fluctuations (power tilts) about a mode that is not the true fundamental mode. This deleterious feedback prohibits the use of batch or Central Limit Theorem approaches which are commonly used in statistical analysis of MC studies. More research is needed to characterize the underlying mechanism of the bias and determine if it is a numerical phenomenon arising from the specific equilibrium xenon algorithms and their numerical implementation within the power iteration algorithm, an amplification of a real physical effect (xenon flattens power distributions), or a combination of both.

These issue prompts a critical question: why simulate real physics, such as xenon effects, if numerical bias arising from user-defined simulation parameters might mask these effects? It emphasizes the importance of establishing appropriate *N* values for accurate representation of reactor behavior in full-core Monte Carlo criticality simulation. The open literature is lacking in the reporting of and documentation of the optimal *N* for the various reactor lattice types under study. The underestimation of apparent variance of local tallies to the real variance is another issue needing more analysis for the different reactor lattices as well as isolating and quantifying the different contributions as a function of *N*; inter-cycle correlation may be only one of several contributions. However, addressing possible bias in the tally means is a more pressing issue especially since this study has identified for the first time the present of bias from multi-physics feedback.

ACKNOWLEDGMENTS

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