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Source Convergence in Monte-Carlo Criticality Simulation of CANDU-6 Reactor

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1. Introduction

Monte-Carlo criticality simulation has been used extensively to estimate the highest eigenvalue (k_{eff}) and the corresponding eigenfunction of the system. The simulation performs essentially a power-iteration method in which the initial fission source distribution guess is iterated over the cycles (or batches/generations) until converged to the fundamental mode before tallying process begins. There are three fundamental limitations must be addressed to obtain correct results:

1. Sufficient initial cycles must be discarded before tallying to ensure the results are not contaminated with the initial source distribution guess [1] and higher modes,
2. Sufficient number of neutron history must be simulated to minimize the random errors and biases in eigenvalue and eigenfunction [1],
3. Ensure the fission source converges to the expected/anticipated distribution (i.e. no particle clustering).

Dominance ratio (DR), defined as the ratio of the highest (k_{eff}) to the second highest (k_1) eigenvalue, describes the source convergence rate during criticality simulation. Therefore, the source convergence rate decreases as the DR closer to unity. For spatially decoupled system (high DR, i.e. 0.99), the simulation requires at least 450 power iterations to minimize the error from higher harmonics to below 1%.

This paper examines the source convergence during the Monte-Carlo criticality simulation of CANDU-6 reactor (high DR system). Section 2 discusses the CANDU-6 model in MCS Monte-Carlo code [2] used in the study. Section 3 discusses the power-method convergence and available diagnostic tools (Shannon entropy and Center of Mass) and their weaknesses and convergence properties. The study examines the source convergence behavior of point- and uniformly-distributed source initial guesses. Biases in reaction rates are manifested in the form of power tilts for cases with smaller number of particles per cycle, despite Shannon entropy metric indicating a converged fission source. In these cases, the fission sources had converged to a stationary distribution that deviated from the true fundamental mode. In Section 4, we propose an alternative approach to minimize the bundle-power biases with Central Limit Theorem (CLT) by merging multiple independent runs (initialized with different random number seeds) of smaller number of particles per cycle. The CLT study also independently confirms "true" fission source convergence for a reference solution using 10^7 particles per cycle.

2. 1/8 CANDU-6 Equilibrium Model

The study uses the 1/8 "equilibrium" CANDU-6 model from previous study [3] in MCS Monte Carlo code. The problem-phase space was reduced by applying reflective boundary conditions assuming conventional quadrant symmetry, and an additional plane-of-symmetry is applied at the core midplane perpendicular to the fuel channels. Figure 1 shows the model geometry and the rectangular fuel-channel lattice (11×11×6) which represents channel rows M-W, channel columns 12-22, and bundle positions 7-12. The material compositions are summarized in Table I.

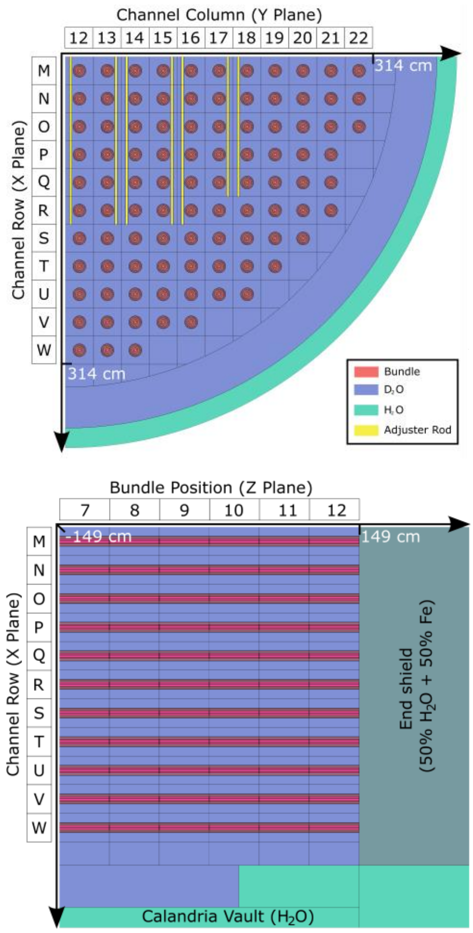


Fig. 1. The cross-section view of 1/8 CANDU-6 model in MCS.

Table I: Material Compositions

Cell	Material	Density (g/cm^3)	T (°C)
Fuel [4]	UO_2 (3.75 MWd/kgHM)	10.420	690
Cladding	Zircaloy-4	6.550	627
Pressure Tube	Zircaloy-2	6.550	227
Calandria Tube			20
Coolant	D_2O (97.5% purity)	0.813	290
Moderator	D_2O (99.8% purity)	1.085	70

The equilibrium term refers to the time- and core-averaged bundle irradiated to 3.75 MWd/kgHM at 450 kW power assuming an average discharge burnup of 7.5 MWd/kgHM for the standard 37-element natural uranium bundle in a CANDU-6 with adjuster rods. All of the 37-element fuel bundles in the model use the equilibrium material composition obtained from a standalone lattice-cell depletion calculation from previous study in [4].

3. Source Convergence

3.1. Power-method Convergence and Diagnostic Tools

The study by [1] describes the convergence of eigenvalue and eigenfunction during the power method as

$$k_{eff}^{(n+1)} = k_0[\,1 - \rho^n(1-\rho)g_1 + \cdots] \qquad (1)$$

$$\phi^{(n+1)} = \phi_0 + \rho^{(n+1)} \cdot \frac{a_1}{a_0} u_1 + \cdots \,, \qquad (2)$$

for n is the cycle number, a_0 and a_1 are constants determined by the expansion of the initial source distribution, u_1 and g_1 are the first higher mode eigenvalue and eigenfunction, ρ is the dominance ratio, and k_0 and ϕ_0 are the fundamental eigenvalue and eigenfunction.

Equations (1) and (2) show that the noise in eigenvalue and eigenfunction from higher harmonics dies off as $\rho^n(1-\rho)$ and $\rho^{(n+1)}$ [1]. Consequently, the k_{eff} will converge faster than the fission source distribution due to the damping factor of $(1-\rho)$ which is close to zero for high DR system. Therefore, it is essential to diagnose the source convergence not only from k_{eff} but also from the source distribution.

This study uses two diagnostic tools available in MCS, namely Shannon entropy and Center of Mass, to examine the source convergence. Shannon entropy H was introduced by [5] to diagnose the source distribution convergence and defined as

$$H^{(n)} = -\sum_{i=1}^{m} p_i^{(n)} \log p_i^{(n)} \,, \qquad (3)$$

for p_i is the fraction of source sites to the total number of particles per cycle in mesh i at start of the cycle n. As fission source converges to the fundamental mode, the entropy is expected to converge and fluctuate about an average entropy value.

The center-of-mass (CoM) technique was introduced in [6] as another diagnostic tool to examine the source convergence. The CoM is expressed by,

$$CoM^{(n)} = \frac{\sum_{i=1}^{N} q_i^{(n)}}{N} \qquad (4)$$

for q_i is the particle i cartesian-coordinate system and N is the total number of particles per cycle.

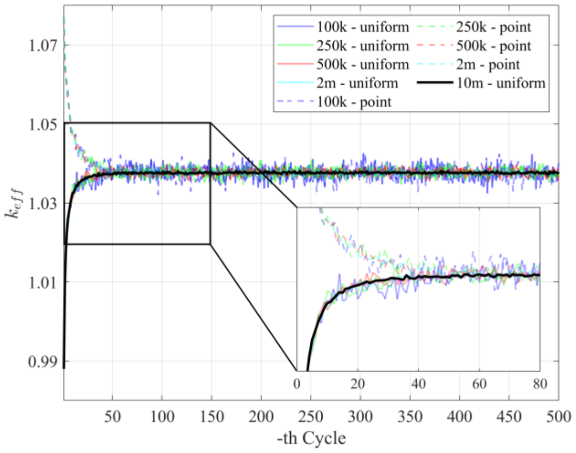
3.2. Initial Source Distribution Guess

In Monte-Carlo criticality simulation, the source distribution (eigenfunction) is not known a priori. Consequently, sufficient initial cycles (referred to as inactive cycles) must be discarded to ensure the results are not contaminated with the errors from initial source distribution guess and higher modes. Therefore, the initial source distribution should be defined as close as possible to the expected distribution to minimize the error contribution from the initial guess and to minimize the required number of inactive cycles.

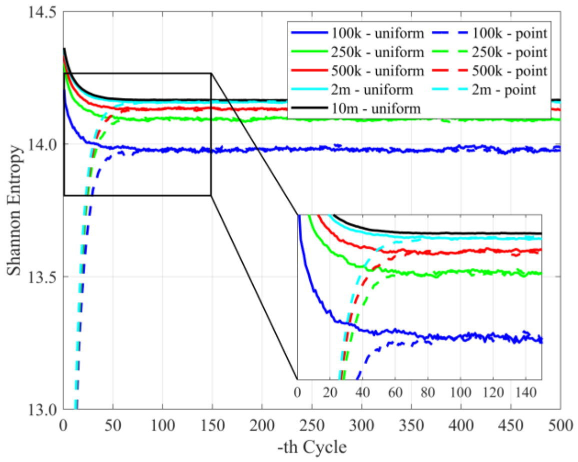
Two initial source distributions are explored in the section: point source at center of the core (bundle row M, column 12, position 7) and uniformly distributed source on all bundles. The simulations were performed with 10^5, 2.5×10^5, 5×10^5, and 2×10^6 particles per cycle for a total of 500 cycles.

Figure 2 shows the evolution of k_{eff} and Shannon entropy during source convergence. As expected, the k_{eff} converges faster than the eigenfunction (here, indicated by the H) due to the damping factor of $(1-\rho)$ in Eq. (1). This behavior is consistent and does not depend on N and number of cycles. Therefore, Fig. 2 reiterates the importance of not relying only on eigenvalue alone to determine the source convergence.

Figure 2b shows that the Shannon entropy of uniformly-distributed-source cases converge faster than the point-source cases. The point-source cases require additional cycles for the particles to migrate from the center of the core [see coordinate (0,0,-149) in Fig. 1] towards the fundamental mode distribution. It is likely that the point-source cases in CANDU-6 simulation migrates faster than of PWR and BWR due to the relatively longer migration length. Unlike the point-source cases, the uniform-source cases require fewer cycles to converge since the initial guess are reasonably close to the converged source. As a result, the uniform-source case is more efficient since it takes fewer cycle to converge. The entropy and CoM in Fig. 2b and Fig. 3 indicate that the uniform cases appear to converge at 60 inactive cycles while for point cases around cycle 70.



(A) The k-eff evolution



(B) The Shannon entropy evolution

Fig. 2. The source convergence of point and uniform initial source guesses compared to the reference case (10^7 particles - uniform). The eigenvalue (k_{eff}) converges faster than the eigenfunction (indicated with H).

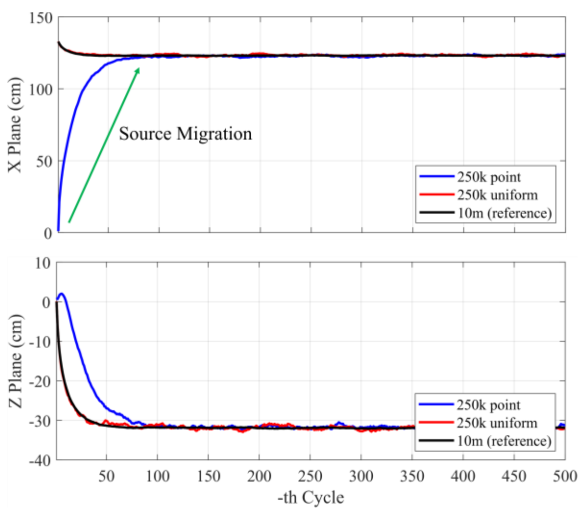


Fig. 3. The evolution of Center of Mass for 2.5×10^5 particles per cycle for both point and uniform cases compared to the reference case (10^7 particles per cycle).

Comparing Fig. 2b to Fig. 3 shows the shortcoming of Shannon entropy. The summation term in Eq. (3) may result in compensation terms which may lead into a false convergence indicator. Although Fig. 2b shows that the 2.5×10^5 point case appears to converge at around cycle 70, CoM in Fig. 3 indicates that the case converged later at around cycle 100 (see Z Plane). Therefore, it is important to determine the source convergence by considering the evolution of both Shannon entropy and CoM.

Overall, it has been demonstrated that the uniform-source cases converge faster than the point-source cases. This behavior is consistent with previous studies conducted in [1], [7]. The subsequent simulations will use uniformly distributed source with 120 inactive cycles to effectively minimize the errors from the initial source guess.

3.3. Source Convergence and Bias in Bundle Power

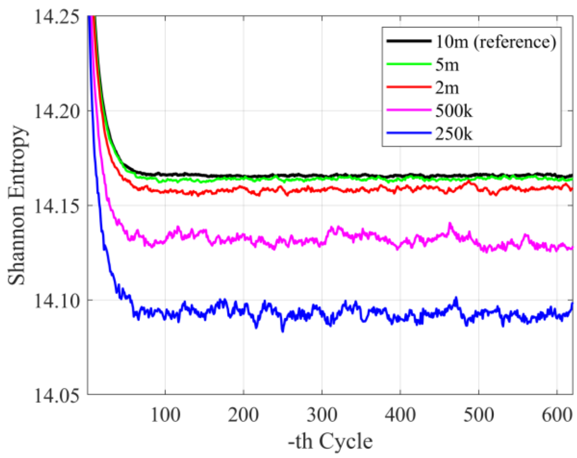
Most Monte-Carlo codes use successive generation method for criticality simulation. During a criticality simulation, the expected number of neutrons produced $E[N_{n+1}]$ after a given cycle is $k_{eff} N_n$. In the successive generation method, the number of neutrons (or alternatively the total neutron weight) of the next cycle must be adjusted by the factor (N_n/N_{n+1}) to maintain constant number of neutrons. However, renormalizing by dividing by a stochastic quantity (N_{n+1}) in each cycle has been shown to introduce a bias in both k_{eff} and any local tallies or distributions. [1], [8]

Studies by [1], [8] established the bias in k_{eff} is

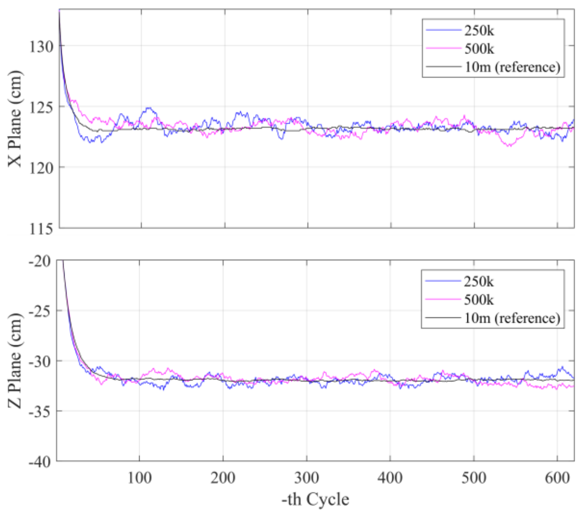
$$\Delta k = -\frac{\sigma_k^2}{k_{eff}} \cdot \sum_{J=1}^{\infty} r_J \propto \frac{1}{N} \tag{5}$$

with σ_k^2 as the computed population variance assuming k_{eff} of each cycle is not correlated and r_J is the lag-J correlation between cycle values of k (r_J are assumed to approach 0 for large J). Based on Eq. (5), the biases in k_{eff} and reaction rate are independent of the total number of cycles but proportional to $1/N$. Therefore, the biases in the results can be minimized by running sufficient number of particles per cycle. Studies by [1], [7], [9] provide demonstration of biases in k_{eff} as a function of N. On the other hand, the biases in reaction rates or components of a reaction rate may be positive or negative. In practice, the widespread availability and reduced cost of computing hardware, e.g., multi-core processors, over the past decade allows the code user to run sufficient number of histories in a reasonable clock time.

The source convergence and potential biases in the bundle powers are investigated by simulating several cases of N for 120 inactive and 500 active cycles with the same Shannon-entropy mesh configuration. Figure 4 shows both Shannon entropies and CoMs indicate the fission source has converged into a stationary distribution for all cases. Assuming the fission source of 10^7 particles per cycle reference case has converged and is an unbiased estimate (or expectation value) with small variance of the true fundamental mode, the average entropy of the reference case represents a single numerical value of the expected fundamental mode source distribution. The cycle-by-cycle Shannon entropies of case 5×10^6 were observed to oscillate closely to the reference case meaning the source distribution of is close to the fundamental mode. Figure 5c confirms that most bundle-power errors calculated with respect to the reference case bundle powers, are effectively minimized to within the statistical uncertainties of the simulation (MCS std).



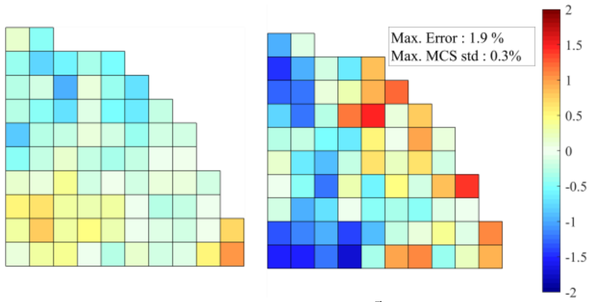
(A) The Shannon entropy evolution



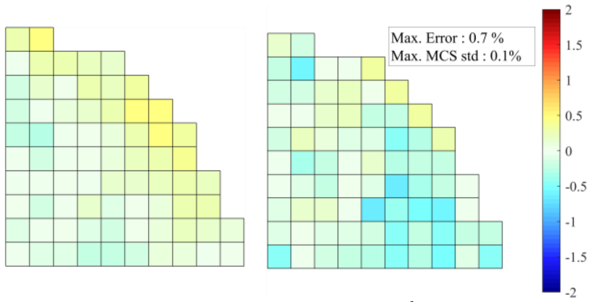
(B) The evolution of Center of Mass

Fig. 4. The source convergence with uniformly distributed source as the initial guess. The entropies of case 2.5×10^5 and 5×10^5 converged to lower value than the reference indicating sources are more concentrated toward specific regions.

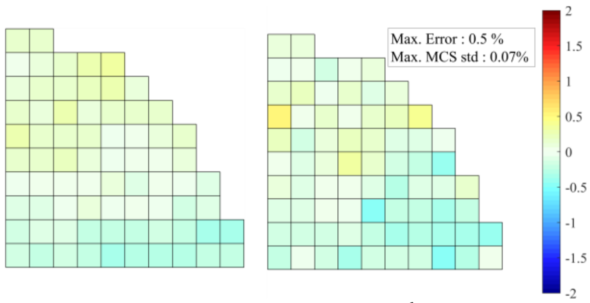
Case 5×10^6 particles per cycle is selected as the "converged" model that can be used in future CANDU research with a factor of two improvement in simulation time with respect to the reference model. The cycle-to-cycle entropy oscillation of the case overlaps with the reference case indicating the 5×10^6 particles per cycle sufficiently samples the phase-space. Furthermore, the converged model satisfies the performance target of less than 0.5% statistical standard deviation for local element powers (the smallest volume over which power is tallied). The converged model gives the maximum absolute standard deviation of 0.029 kW (0.0012% relative standard deviation) for element at bundle M-12 position 8 (high-power bundle) while the largest relative standard deviation is 0.5% (0.0049 kW) for element at bundle Q-21 position 12 (low-power bundle).



(A) Errors of Case 2.5×10^5 (seed 1)



(B) Errors of Case 2×10^6



(C) Errors of Case 5×10^6

Fig. 5. The bundle-power errors of case (A) 2.5×10^5, (B) 2×10^6, and (C) 5×10^6 at position 7 (left) and 12 (right). The bundle power errors are calculated with respect to the reference case. Most bundle errors of case 2×10^6 and 5×10^6 are within their respective simulation uncertainties (MCS std).

The entropy and CoM convergence indicates the fission-neutron sources have converged into a stationary distribution–often assumed to the fundamental mode–which can give a misleading interpretation [10]. The stationary distribution may be deviated from the fundamental mode giving biases in the results. Figure 4a shows the entropies of cases with smaller N converge to lower average entropy values than the higher N cases, providing an indication of potential biases in the reaction rate (represented by bundle power). For the same Shannon-entropy mesh configuration, the maximum entropy value is obtained when the sources are evenly distributed in the mesh (see H at cycle 0 in Fig. 4a) while the minimum value is achieved when the source is concentrated in a single point of space (see H of point cases at cycle 0 in Fig. 2b). So, the source distribution of cases with smaller N are more concentrated towards specific regions of the system than the reference case. Consequently, the sources in the concentrated regions are likely to induce more fission reactions in the neighboring bundles (overestimation) while underestimate bundle powers of less concentrated regions. Therefore, it is likely that we will observe the biases in a form of power tilt for the lower N cases.

Figure 5a confirms the biases in reaction rate is manifested as a significant power tilt between the quadrants in center of the core and bottom of the core. Later in Section 4, we perform CLT study to investigate whether the biases will be compensated by merging multiple independent runs of 2.5×10^5.

4. Cancellation of Bundle-Power Biases with Central Limit Theorem

There are two independent unbiased estimates of the true bundle powers, each with accompanying confidence intervals quantified by standard deviations. Assuming the fission-source distribution is fully converged for the 10^7 case, the bundle-power tallies and accompanying Monte-Carlo standard deviations are unbiased estimates of the true bundle powers. According to the CLT, the sample means of independent and identically distributed draws from a population are normally distributed as the number of samples becomes large, and the mean of this distribution is an unbiased estimate of the true population mean. The results from Monte-Carlo simulations initialized with different random seeds are analogous to random draws from a population. Here we hypothesize tally results from multiple simulations with small N, each which have a biased or tilted power distribution but these biases are random being conditioned on the random number strides generated from the different seeds, can be analyzed with the CLT. Therefore, aggregated tally results from multiple runs should also be unbiased estimates of the true bundle powers and are independent of the reference case results.

Multiple independent runs of the 2.5×10^5 case are used in the CLT study. The aggregated tally results are examined to determine whether the biases among the runs cancel each other. Section 3.3 establishes the biases are manifested in the form of power tilts for smaller N cases. We suspect that the power tilt locations may vary simulation-to-simulation due to the random nature of a Monte-Carlo simulation. Comparing Fig. 5a and Fig. 6 confirms that the power tilt locations at bundle position 12 differ simulation-to-simulation. Therefore, this behavior indicates the possibility of cancellation of biases for the bundle power by merging multiple independent runs of smaller N.

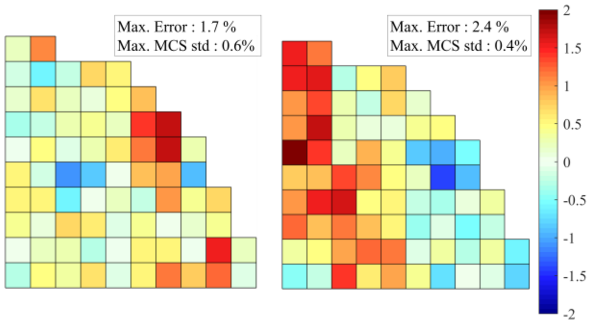
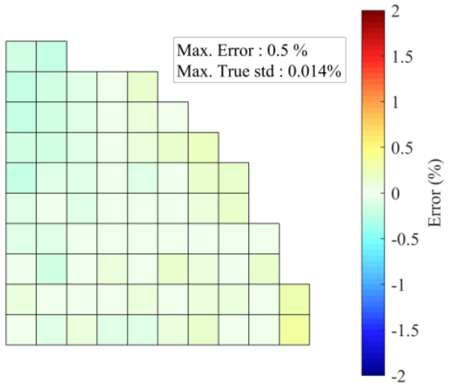
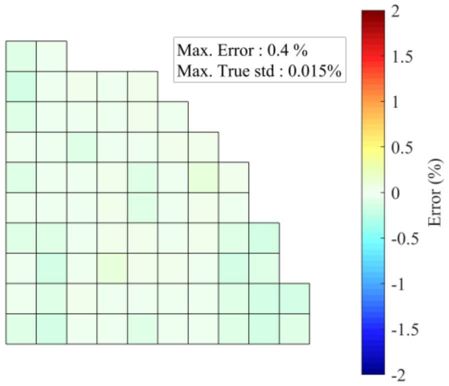


Fig. 6. The bundle power errors of case 2.5×10^5 at position 12 for seed 847 (left) and seed 45 (right). The power tilt locations varied simulation to simulation.



(A) Merged bundle powers from 20 independent runs



(B) Merged bundle powers from 100 independent runs

Fig. 7. The bundle-power errors from merging 20 and 100 independent runs of 2.5×10^5 particles per cycle. The bundle power errors are calculated with respect to the reference case. The biases are effectively minimized by merging multiple independent runs.

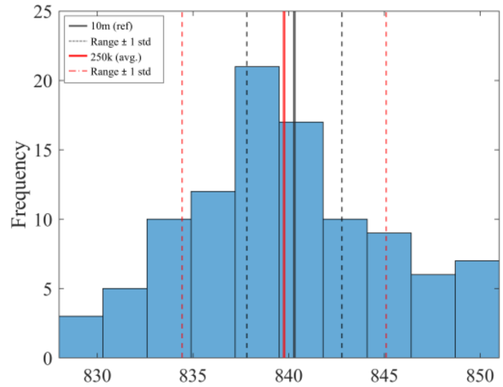
Figure 7 shows the bundle-power errors at position 7 by merging 20 and 100 independent runs (the 20-run sample is included as the first 20 runs in the 100-run sample). The sample standard deviation is calculated from the CLT by

$$\sigma_b = \sqrt{\frac{\sum_{i=1}^{M}\left(P_{b,i} - \overline{P_b}\right)^2}{M-1}}, \tag{6}$$

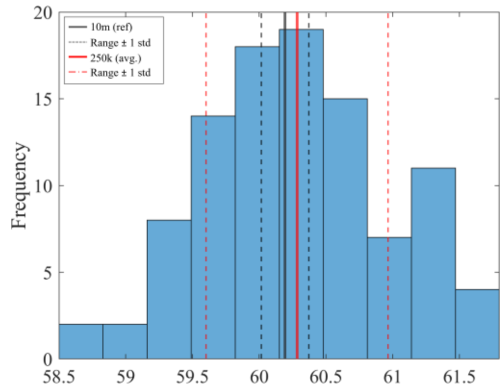
with the average bundle power defined as

$$\overline{P_b} = \frac{\sum_{i=1}^{M} P_{b,i}}{M}, \tag{7}$$

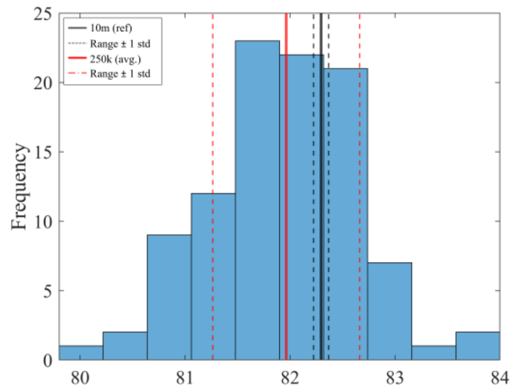
where M is the number of independent simulations and $P_{b,i}$ is a bundle power from the i^{th} simulation.



(A) Bundle M-12 Position 7 (highest power)



(B) Bundle M-22 Position 12 (lowest power)



(C) Bundle W-13 Position 12 (largest error)

Fig. 8. The bundle power variation from 100 independent runs of case 2.5×10^5 with different random number seeds. The merged bundle power (red solid lines) closely match the bundle power of the reference case (black solid lines).

As suspected, the biases from the independent runs cancel each other due to the variation of power tilt locations simulation-to-simulation. Furthermore, the errors in Fig. 7a derived from 20 simulations each using 500 active cycles times 2.5×10^5 particles per cycle and Fig. 5c using one simulation with 500 active cycles times 5×10^6 particles per cycle are comparable noting that both cases used equivalent number of simulated particles (2.5×10^9 particles).

Figure 8 shows the variation in bundle power from 100 independent runs follows the normal distribution predicted by the CLT. The average bundle power (red solid line) closely matches the bundle power of the reference case (black solid line). Figure 8a and 8b show that both bundle power of the reference study and the average bundle power fall within each other's confidence interval for the highest and lowest bundle power. The largest error is observed in Fig. 8c to be 0.4% (0.3 kW) at bundle W-13 position 12 where the merged bundle power falls outside of the reference confidence interval (black dashed line).

The CLT provides a quick independent approach of obtaining unbiased estimates of the bundle powers while minimizing the biases manifested in the bundle powers encountered in a single small N case. Furthermore, merging multiple independent runs is shown to address the uncertainties underestimation in Monte-Carlo criticality simulation (see [1]). Rather than running a single simulation of the converged model which takes 5 days in the 64-core cluster used in this study, the user may seek the CLT approach by accumulating completed shorter simulations to get rough estimates of how the reaction rate/power distribution looks like. Furthermore, we observed the total simulation time of the 20 runs is 15 hours faster than the converged model simulation time.

5. Conclusions

The study investigated the source convergence in Monte-Carlo criticality simulation of CANDU-6 reactor and established 120 inactive cycles, 500 active cycles, and 5×10^6 particles per cycle are the simulations parameters that give a fission source that is converged to the true fundamental mode for the 1/8 CANDU core with adjustor rods modeled. Shannon entropy and CoM metrics can give "false convergence" when the fission source converges to a stationary distribution that deviates from the fundamental mode distribution if an insufficient number of particles per cycle are simulated. The false convergence runs have lower Shannon entropy values than a truly converged simulation when using identical Shannon entropy mesh indicating local regions of concentrated fission density. For the CANDU core model case, the CLT approach of merging tallies from multiple runs of low particles-per-cycle initialized with different seeds appears to eliminate the power tilts and biases present in the individual runs as well as providing an independent check of the true fission source convergence for a reference solution using a very large number of particles per cycle. In future work, the CLT approach performance should be tested for other reactor types with different underlying physics (e.g., thermal-spectrum PWR and fast reactor) and for full-core calculation with equilibrium xenon algorithm activated.

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