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Preliminary Analysis of True Variance of Local Power Tallies in Monte Carlo Simulation of Fast Spectrum Reactors

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1. Introduction

In Monte Carlo criticality simulations, a power-iteration method is performed where the initial fission source distribution guess is iterated over inactive cycles until convergence to the fundamental mode after which the tallying process occurs during active cycles. In a large geometry problem with slow convergence rate (typically with high dominance ratio close to 1), one requires enough number of inactive cycles and a very high number of particles per cycle in order to achieve fission source convergence and to properly incorporate detailed distributions of sub-pin level local tally profile. However, the use of random numbers makes the calculation results statistically fluctuate even after fission neutron source distribution has converged. Furthermore, inter-cycle correlation exists as the fission sites in the previous cycle are used as neutron generation sites in the following cycle which makes tally realization between cycles closely related and not independent leading to variance bias where apparent standard deviation (the standard deviation calculated by the Monte Carlo code and output with the tally mean) of a local tally is smaller than the 'true' standard deviation. In a high dominance ratio problem with slow convergence rate where the inter-cycle correlation is stronger, the statistical error generated in the preceding cycles are propagated and accumulated through the fission source distribution causing a more severe variance underestimation bias and eventually a systematic error [1–5].

The variance of a Monte Carlo tally is ideally inversely proportional to the number of simulated particle reaction rate in the condition that tally realizations are uncorrelated. However, the existence of inter-cycle correlation can reduce the convergence rate of the statistical error below the ideal behavior. Most production Monte Carlo codes calculate tallies and their variances assuming no correlation for the local tally estimation, thus the effect of inter-cycle correlation on local tally uncertainty is essentially ignored making the apparent standard deviation smaller than the real standard deviation [5–7].

Previous studies also observed that the variance bias for assembly-wise tallies is larger than bias for local (pin-wise) tallies [4,8]. One explanation for this phenomenon is that smaller tally regions have lower auto-correlation coefficients [9]; therefore, assembly auto-correlation coefficient is strongly positive as it is the summation product of positive auto-correlation coefficient of all neighboring pins in that assembly [8] causing a more severe underestimation of tally standard deviation. Another explanation is that if the computational mesh is large enough such that a neutron has a lower probability of escape from the mesh, then the next generation fission neutrons will be generated in the same mesh with a greater probability; therefore, the inter-cycle correlation becomes greater with a larger mesh size and consequently the variance bias becomes larger [4]. Another source of positive auto-correlation between neighboring pins arises at the particle history level from the use of implicit absorption variance reduction technique which is default in most production Monte Carlo codes. In a real reactor, a single neutron can only induce a fission event in a single discrete location—the neutron only contributes to the power in a local volume around the fission site—but in implicit absorption, the neutron is never actually absorbed. The neutron weight is decreased (or increased if it survives a roulette call) and can escape the fuel pin and enter a neighboring pin and contribute to that power tally. In fixed-source simulation of an accelerator-driven subcritical CANDU core, this effect for 37-element fuel bundle power tally can be as high as a factor of six underestimation if the element powers are assumed to be independent [10].

Practically all of the aforementioned variance bias studies were performed with full-core pressurized water reactor models or idealized benchmarks (usually light-water reactor related). Full-core Monte Carlo analyses of other reactor types with (significantly) different neutron transport properties, such as fast reactors, are becoming more prevalent and even being applied in engineering design, regulatory compliance, and licensing calculations. The basic research question that motivated the current study is: how much of the local tally variance bias is a numerical property of the power-iteration method employed in Monte Carlo criticality simulations and how much is an artifact of the underlying neutron transport physics of the studied test cases? To address this question, more reactor types need to be studied and the real-to-apparent standard deviation ratios quantified for local power tallies for these cores.

This study is a first attempt to obtain pin-wise and assembly-wise local power tally ratios for a fast spectrum reactor test case. Section 2 introduces the fast reactor model employed in the study and establishment of Monte Carlo simulation parameters, number of inactive cycles and number of histories per cycle that ensure convergence k_{eff} and Shannon entropy. In section 3, the true variance of pin-wise and assembly-wise power tallies are estimated from the "batch method" where 100 independent criticality simulations initialized with different random number seeds are performed for each combination of total number of simulated particles N_{tot} (number of active cycles times the number of particles per cycle) and the number of particles per cycle.

2. The 2D R-θ Fast Reactor Model and Monte Carlo Simulation Parameters

An LBE-cooled, UO_2-fueled fast reactor core model based on the fuel lattice parameters of MicroURANUS [11] and used in a previous study [12] is selected. Figure 1 shows the radial enrichment zoning which gives a flat power distribution (high dominance ratio), and the 50-cm thick radial reflector is a 50%/50% mixture of stainless steel (SS) and LBE. The active core diameter is 150 cm, so this core is physically large for a representative fast reactor, so some spatial decoupling of the inner core and outer core driver fuel zones exists. The assembly height is 2 cm effectively reducing the core to a 2D R-θ model. Reflecting boundary conditions are applied on all sides except for black/vacuum condition at the outer radius of the reflector making the R-θ model an accurate surrogate of an axially symmetric 3D core at the mid-plane.

The benchmark pin-power distribution is obtained from a simulation using 5M particles per cycle and 100 inactive cycles and 500 active cycles. All simulations use a uniform initial fission source distribution to initialize the inactive cycles. Figure 2 shows the Shannon entropy and k_{eff} convergence plots for varying particles per cycle. The 2M case converged Shannon entropy oscillates with the 5M benchmark while lower particles per cycle cases show larger cycle-to-cycle fluctuations and a lower asymptotic Shannon entropy value. The previous study [13] found through visual inspection of Shannon entropy and Center of Mass plots that twenty inactive cycles are required for fission source convergence, so 25 inactive cycles parameter is used for all simulations in this study.

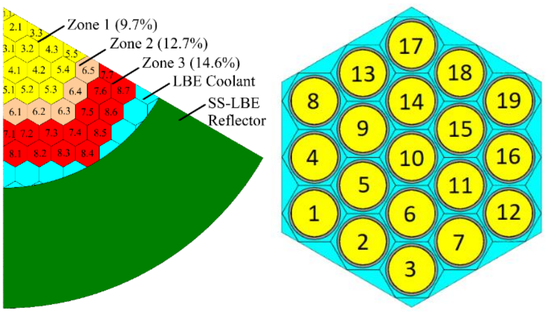

Fig. 1. Left: R-θ core model with 3 enrichment zones; Right: Fuel pin indexing in fuel assembly.

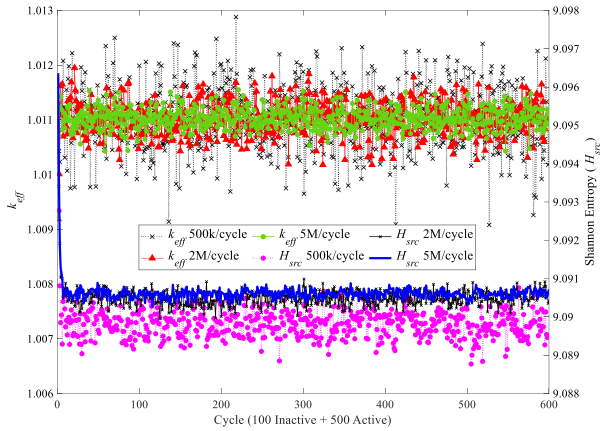

Fig. 2. Criticality (k_{eff}) and Shannon entropy (H_{src}) plot shows 2M particle per cycle adequately mimics the 5M particle per cycle.

3. Results and Discussion

3.1. Results From Simulations Using Twenty Million Total Particles

Preserving N_{tot} of 20M in a single criticality simulation, three cases varying the number of particles per cycle (100k/cycle, 500k/cycle, and 1M/cycle) are considered. Each case consists of 100 independent simulations with 553 fuel pin fission reaction rate tallies and 32 fuel assembly fission reaction rate tallies (power tallies). Figure 3 shows that the averaged values of local pin power tallies obtained from 100 simulations are in close agreement with the benchmark pin powers regardless of the number of particles per cycle used, indicating the stochastic fluctuations of the fission source and power distributions during active cycles average out when combining independent runs. The true standard deviations (+/-1σ error bars in Fig. 3) are calculated from the sample standard deviations of the individual mean pin powers. The pin power true variances appear to be insensitive to the number of particles per cycle.

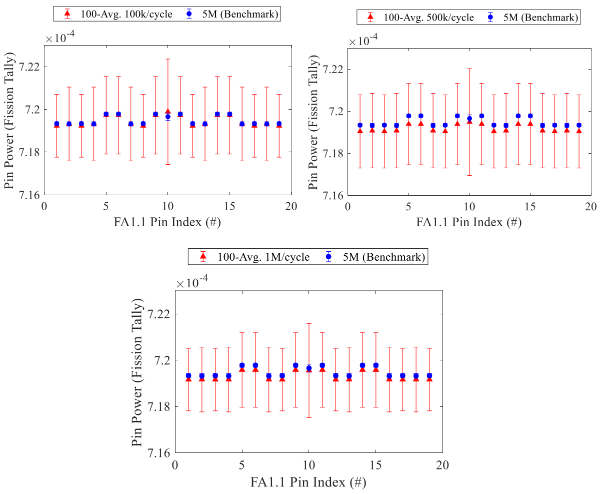

Fig. 3. FA1.1 mean pin powers for particle per cycle cases that simulate twenty million total particles. The +/-1σ error bars are estimates of the true standard deviations obtained from the sample variance of the pin power data from 100 independent simulations.

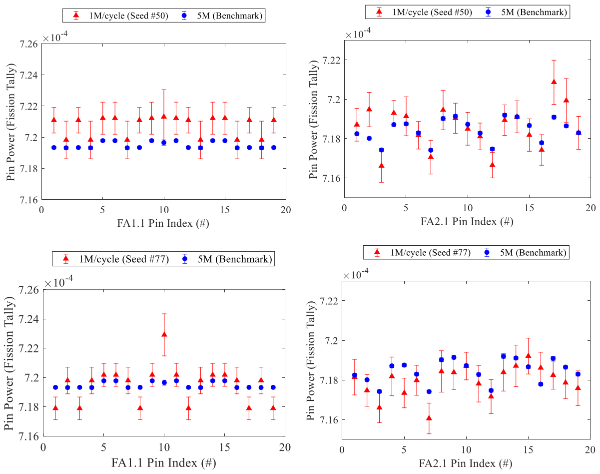

Fig. 4. Pin power estimates and associated apparent standard deviations from single Monte Carlo simulations using 1M/cycle. Seed #50 (Top) and Seed #77 (Bottom) cases in FA1.1 (Left) and FA2.1 (Right) relative to benchmark value.

Figure 4 shows the pin powers and apparent standard deviation tally results from single Monte Carlo simulations drawn from the 100-simulation dataset using 1M particles per cycle. From simulation-to-simulation, the sign and magnitude of the pin power errors relative to the benchmark solution can fluctuate. Some pin power relative errors are large enough that the benchmark pin power lies in the tail of the confidence interval defined by the simulation mean and apparent standard deviation.

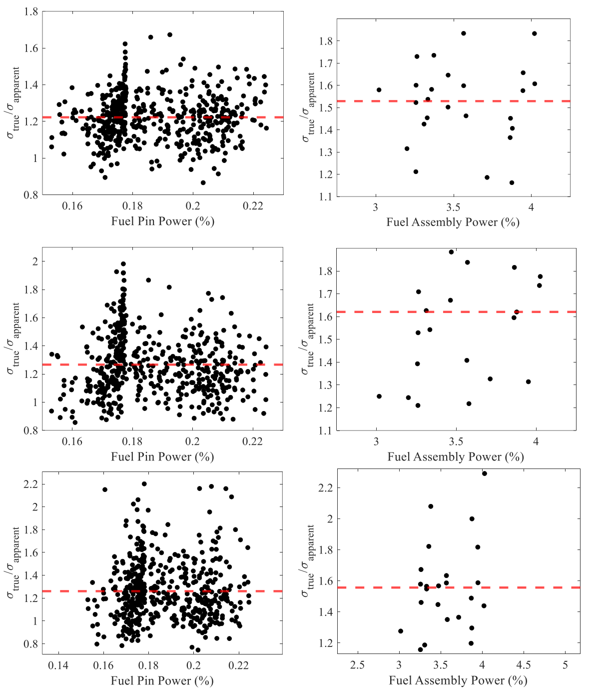

Fig. 5. The fuel pin and fuel assembly $\sigma_{true}/\sigma_{apparent}$ ratio plots and average ratio (red dashed line) for select N_{tot} = 20M cases. Top row: 100k/cycle (Seed #38); Middle row: 500k/cycle (Seed #99); Bottom row: 1M/cycle (Seed #50).

Figure 5 shows the true-to-apparent standard deviation ratio distribution and its average value (red dashed line) from an arbitrary simulation sample drawn from each case dataset. Sample statistics using all tallies in all simulation by case are tabulated in Table I. Average pin-wise ratios (both the average of 553 ratios from a single simulation and average of 55,300 ratios in a case sample) appear to be consistent and insensitive to the particles per cycle. This insensitivity appears to hold for assembly-wise average ratios and the assembly-wise ratios are larger than the pin-wise ratios which is directionally the same as previous PWR studies [4,8,9,14]. The fast reactor assembly-wise ratios are smaller than the PWR assemblies which can likely be attributed to the neutron transport physics (larger mean-free-path and migration length in the fast reactor). The only present trend is the increase in ratio variance as the number of particles per cycle is increased. This trend is most likely due the lower number of active cycles for higher number of particles per cycle to preserve N_{tot} which affects the calculated tally standard deviation to have a wider distribution. Another interesting thing is that some pin-wise ratios are less than unity indicating the apparent variance is overestimating the true variance. However, as the true variance is the average from 100 simulations, it is expected that some apparent variances to be larger than the true variance due to the stochastic process in the simulations. The reflecting boundary conditions used in this 2D model could be contributing to these behaviors, thus, future work will test a 3D fast reactor core.

Table I. True-to-Apparent Standard Deviation Ratio Statistics from 100 simulations of N_{tot} = 20M cases.

N_{tot} = 20M	Ratio Avg.	Ratio Std.	Min/Max Value
Case	Pin-Wise Power Tallies		
100k/cycle	1.23	0.13	0.79/1.84
500k/cycle	1.26	0.21	0.71/2.79
1M/cycle	1.25	0.25	0.62/3.00
Case	Assembly-Wise Power Tallies		
100k/cycle	1.55	0.18	1.06/2.14
500k/cycle	1.61	0.31	0.93/3.11
1M/cycle	1.55	0.31	0.76/3.05

3.2. Results From Simulations Using One Million Total Particles

Preserving N_{tot} of 1M in a single criticality simulation, three cases varying the number of particles per cycle (10k/cycle, 50k/cycle, and 100k/cycle) are considered. Figure 6 shows that the average pin power tallies are in close agreement with the benchmark pin powers, and the true standard deviations are insensitive to the number of particles per cycle, but the true standard deviations are larger than the 20M N_{tot} results because fewer total particles have been simulated. Figure 7 shows the pin powers and apparent standard deviation tally results for select simulations.

Figure 8 shows the true-to-apparent standard deviation ratio distribution and its average value (red dashed line) for select samples and sample statistics using all tallies are tabulated in Table II. The average ratios are consistent with the 20M N_{tot} results, but the variances of the ratios are larger. The magnitude of the outliers is also larger which can be expected for lower number of total simulated particles.

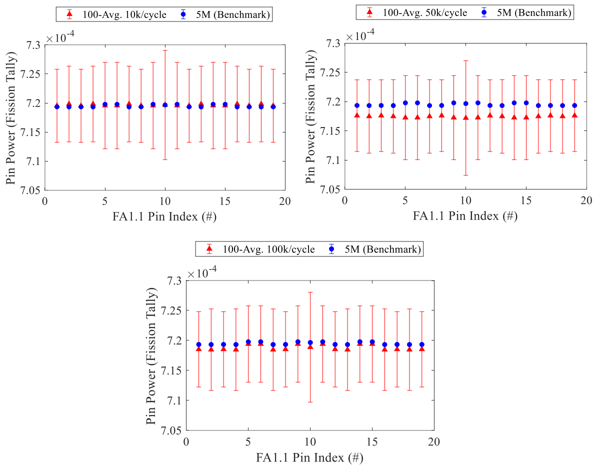

Fig. 6. FA1.1 mean pin powers for particle per cycle cases that simulate one million total particles. The +/-1σ error bars are estimates of the true standard deviations obtained from the sample variance of the pin power data from 100 independent simulations.

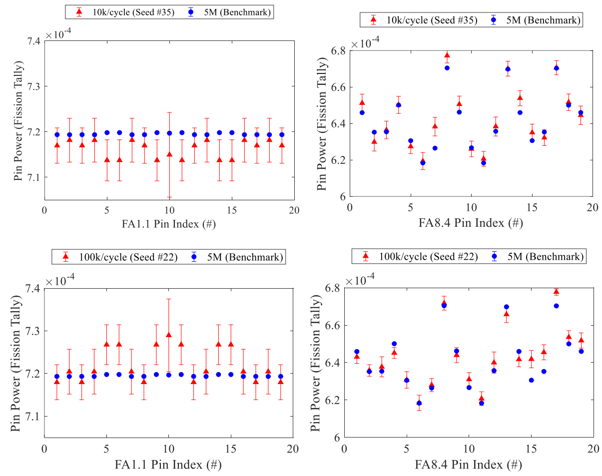

Fig. 7. Pin power estimates and associated apparent standard deviations from single Monte Carlo simulations using 10k/cycle Seed #35 (Top) and 100k/cycle Seed #22 (Bottom) in FA1.1 (Left) and FA8.4 (Right) relative to benchmark value.

Table III. True-to-Apparent Standard Deviation Ratio Statistics from 100 simulations of N_{tot} = 1M cases.

N_{tot} = 1M	Ratio Avg.	Ratio Std.	Min/Max Value
Case	Pin-Wise Power Tallies		
10k/cycle	1.26	0.16	0.74/2.04
50k/cycle	1.22	0.23	0.59/3.64
100k/cycle	1.30	0.38	0.55/5.72
Case	Assembly-Wise Power Tallies		
10k/cycle	1.61	0.21	1.16/2.56
50k/cycle	1.49	0.30	0.71/3.01
100k/cycle	1.63	0.49	0.58/4.16

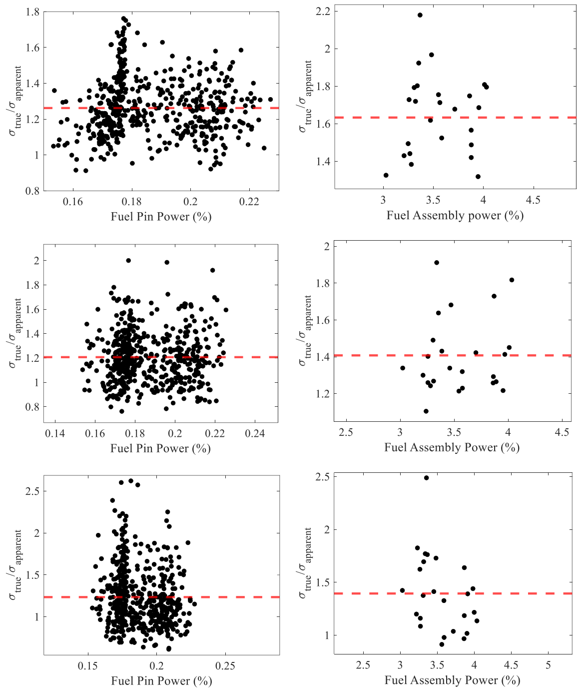

Fig. 8. The fuel pin and fuel assembly $\sigma_{true}/\sigma_{apparent}$ ratio plots and average ratio (red dashed line) for select N_{tot} = 1M cases. Top row: 10k/cycle (Seed #35); Middle row: 50k/cycle (Seed #69); Bottom row: 100k/cycle (Seed #22).

4. Conclusion

Variance bias does inherently exist in current Monte Carlo criticality simulation codes. Lots of previous studies regarding variance bias were performed with light-water reactor models or idealized benchmarks, thus, this study attempted to observe variance bias in another type of reactor: fast spectrum reactor. Using the "batch method" of 100 independent simulations with different random seeds to estimate the true variance of local tallies, we found several notable behaviors in this fast reactor model. First, the true variance is insensitive to the number of particles per cycle when preserving the same total simulated particle (N_{tot}), thus, only by increasing the N_{tot} that the true variance can be reduced. In a rough comparison to the PWR-2D problem in previous study [14] which has ~3.1 true-to-apparent ratio on average, this fast reactor model has a relatively much smaller variance bias with only ~1.3 true-to-apparent ratio for fuel pin case and ~1.6 for the fuel assembly. Next, the assembly-wise variance bias is generally larger than pin-wise variance bias which is a similar behavior in previous studies of LWR-based model [4,8]. True-to-apparent ratio statistics also show an increasing trend of true-to-apparent ratio distribution variance (and the spread of min/max ratio value) as the number of particles per cycle is increased due to the lower number of active cycles to preserve N_{tot} for the higher particles per cycle cases. Lastly, some pin-wise ratios are less than unity because the true variance is the average of 100 apparent variances resulted from a stochastic process, thus, it is expected to have true-to-apparent ratio less than unity.

Further and more detailed study is needed to investigate these variance bias behaviors in fast reactors, such as by calculating and analyzing correlation coefficients between neighboring pin-wise and assembly-wise tally.

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