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Author(s): Bennett, Alexander S.
Kiedrowski, Brian C.
Brown, Forrest B.

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Bias and Uncertainty Under-Prediction in MCNP6.1 Lattice Physics Calculations with Depletion

[1]Alexander S. Bennett, [2]Brian C. Kiedrowski, [2]Forrest B. Brown

[1]*Dept. of Mechanical & Nuclear Engineering, Penn State, 137 Reber Building, University Park, PA 16802,*
[2]*X-Computational Physics Division, Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, NM 87545,*
asb241@psu.edu

INTRODUCTION

The ability to perform Monte Carlo depletion using CINDER90 was implemented in MCNPX about five years ago [1], and this capability has been migrated into MCNP6.1 [2]. This capability is used to study the effects of bias and uncertainty under-prediction in Monte Carlo depletion calculations. Monte Carlo criticality calculations have particular issues that have been known since the 1970's [3, 4]. The first is bias in the results, which is a consequence of using a finite number of random histories to perform a renormalization between cycles of the power iteration. It was shown mathematically in the 1980's that the bias in the effective multiplication k is always negative and proportional to the inverse of the batch size [5]. More recent work has shown that in reactor-type problems, using too small of a batch size can introduce an artificial tilt in the predicted flux shape [6]. The second issue involves not the answers, but the calculated uncertainties, which are too small (i.e., the code states the result is more certain than it actually is) because positive correlation between cycles is neglected [4].

Until now, these effects have only been analyzed for the static case, not one where the results of the Monte Carlo calculations are used for depletion over time. For the case analyzed, a lattice of 2-D assemblies from a Boiling Water Reactor (BWR) computational benchmark, bias did not exhibit a statistically significant effect. The under-prediction of the uncertainties was small, with the exception of the capture rate in localized burnable poisons.

CALCULATION MODEL

A 2-D assembly of a BWR computational benchmark from the OECD/NEA Burnup Credit Expert Group Phase IIIB [7] was used as a template for these calculations. The benchmark assembly is infinitely reflected, containing an 8 $\times$ 8 array of pins with the center four replaced with a water channel. The fuel pins have four different enrichments, and eight of the pins contain gadolinium as a burnable poison. Each fuel pin is modeled as a separate material and the gadolinium pins are further segmented into ten radial zones for depletion. Because this benchmark was too small neutronically to study the effects of bias and uncertainty under-prediction, this assembly was replicated into a 4 $\times$ 4 array, with B_4C control blades between them, as shown in Fig. 1. The boundaries are still reflective.

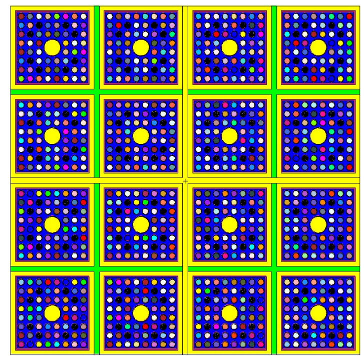

Fig. 1. Geometry model of the 4 $\times$ 4 BWR array.

The MCNP input file was created with a Python script, with the "like but trcl" capability for defining the geometry. As a consequence of creating the geometry this way, MCNP6.1 reserves an exceedingly large amount of memory for new surfaces that made it impossible to run the problem as defined on the 32 GB node available on the Moonlight cluster at Los Alamos National Laboratory (LANL). Modifications had to be made to MCNP6.1, and hopefully the lessons from this can be applied to improving the code in a future release.

The burnup was done at a power of 192 kW. The depletion time steps are: a step 1 day at full power to account for the burn-in of ^{135}Xe , 12 steps at full power of 90 days, and 1 step at no power for 5 years. Tallies were placed in the pins along the diagonal of the problem (lower-left to upper-right). These tallies are the fission of ^{235}U and ^{239}Pu and the capture of ^{238}U , ^{239}Pu , ^{135}Xe , and ^{157}Gd .

RESULTS

Bias

To find the effect of bias, two sets of calculations were run. The reference case uses 10,000 neutrons per cycle for 100 cycles per burnup time step. The biased case uses the same number of overall neutrons (on average), but with 100 neutrons per cycle for 10,000 cycles. The batch size for 10,000 was selected to be sufficiently large such that bias is insignificant; this decision was based on the results in Ref.

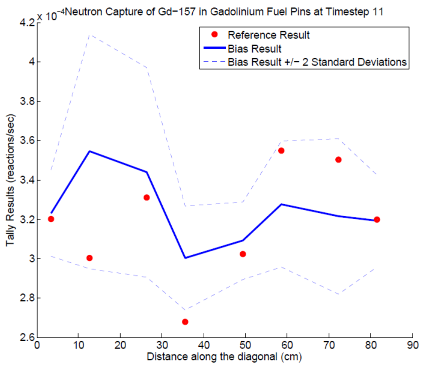

Fig. 2. Comparison of reference and biased results for ^{157}Gd capture.

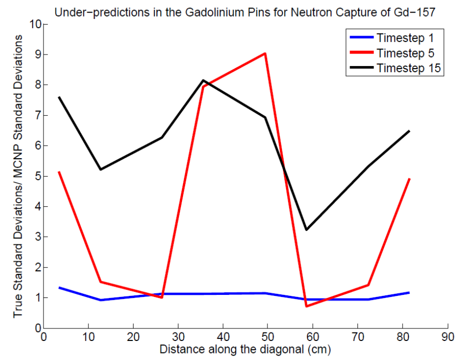

Fig. 3. Uncertainty under-prediction for ^{157}Gd capture as a function of space at various time steps.

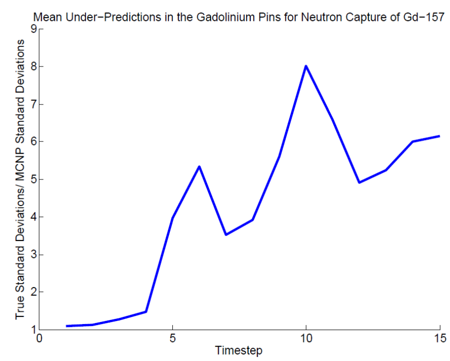

Fig. 4. Uncertainty under-prediction for ^{157}Gd capture as a function of time averaged over all space.

[6]. To improve the statistical accuracy of the calculations, 25 independent cases each using a different random number were run; unfortunately, the biased case only used 23 because two of the continue run dump files were corrupted during the numerous overwrites. The calculations were run with 16 OpenMP threads on the Moonlight cluster at LANL with the each reference case taking 140 hours (wall-clock) and the bias case taking 240 hours. ENDF/B-VII.0 cross sections were used. The calculations were shown to be converged based on convergence of the Shannon entropy.

To evaluate bias, the mean results from the biased case were compared to those from the reference case. For this problem, there was no observed statistically significant difference between the two results, as judged by a 2-σ confidence interval. The case with the largest discrepancy, capture in ^{157}Gd as a function of position along the diagonal at time step 11 is shown in Fig. 2, and all but one of the results is inside 2σ.

Unfortunately, this does not show that bias is not exacerbated by Monte Carlo depletion; rather, it is not for this problem. This problem may have been too small or too symmetric to exhibit a tilt in the flux shape seen in Ref. [6], and further studies are needed to establish a more general conclusion. This does suggest, however, that for simple assembly-level calculations, the effect of bias is probably negligible even for very small batch sizes.

Uncertainty Under-Prediction

To evaluate how well or poorly the uncertainties on the results are estimated, the ratio of the empirical to the reported uncertainties was taken. The empirical uncertainty was obtained by finding the standard deviation of the results for the 25 independent cases (reference cases with 10,000 neutrons per cycle for 100 cycles) regardless of the statistical uncertainties that MCNP calculates. The reported uncertainty is the average of the 25 uncertainties (reference cases again) produced by MCNP.

The tally with the largest under-prediction of the uncertainties is the capture in ^{157}Gd, which appears to grow with time step. None of the other tallies obtained showed any significant under-prediction or trend with time. The spatial dependence along the diagonal is shown in Fig. 3 at time steps 1, 5, and 15. The temporal dependence (averaged spatially over the diagonal each time step) are given in Fig. 4. The magnitude of the under-prediction appears to be negligible at the beginning of life, but grows substantially as the gadolinium burns out, which occurs around time step 5, and then steady increases from then on. After the gadolinium burn-out, the uncertainties are underestimated by a factor of between 5 to 10 – for example, an uncertainty reported as 5% should really be somewhere between 25-50%.

Unfortunately, 25 independent cases is not enough to statistically resolve the uncertainties, since they too are random, so more independent cases are needed for a better quantitative comparison. Nonetheless, the trend observed

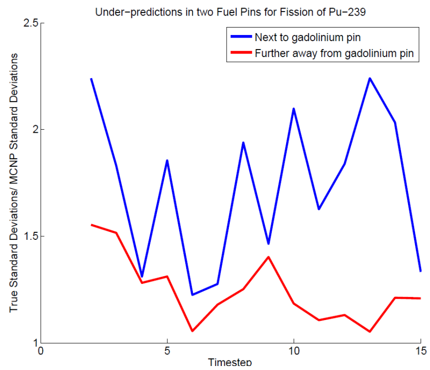

Fig. 5. Uncertainty under-prediction for ^{239}Pu fission as a function of time with different proximity to burnable poison (gadolinium) pin.

in the ^{157}Gd capture is clear, suggesting that burnable poisons are particularly prone to having their uncertainties underestimated (based on the results from the previous section, it may be that for a more difficult problem, the depletion of burnable poisons may also be biased as well). To test if proximity to the gadolinium pins exacerbates the effect for other quantities, the under-prediction the uncertainties as a function of time for fission of ^{239}Pu are obtained for two pins: one adjacent to the gadolinium pin, and another farther away. These results are shown in Fig. 5, and it appears that proximity to the burnable poison has a small, but noticeable impact on the localized under-prediction of the uncertainty.

SUMMARY & FUTURE WORK

An OECD/NEA Burnup Credit Expert Group BWR depletion benchmark was adapted to analyze the effects of bias and uncertainty under-prediction in Monte Carlo depletion. For the small and symmetric problem analyzed, no statistically significant impact of bias was found even for a very small batch size of 100 particles per cycle. This suggests bias of the results is not a significant concern for assembly level calculations. The uncertainties of capture in ^{157}Gd are significantly underestimated because spatial and/or temporal correlation is neglected, and the magnitude of this under-prediction grows with time. Results also suggest that proximity to burnable poisons also has an effect as well, i.e., the closer the greater the under-prediction. For this problem, none of the other reactions looked at had a significant under-prediction of uncertainties.

The next step is to try a larger problem, or at least one with less symmetry. To go bigger, either a different code is needed, MCNP6 needs to be improved to handle larger problems, or a computer with a larger amount of RAM ($>$ 32 GB) is needed. Given this, the effect of the tilt observed in Ref. [6] on depletion can be analyzed to see whether the answers become further biased or some other effect such as spurious xenon oscillations arise.

ACKNOWLEDGMENTS

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