Under-Prediction of Localized Tally Uncertainties in Monte Carlo Eigenvalue Calculations

Brenden Mervin, Scott Mosher, John Wagner, Ivan Maldonado

The University of Tennessee, Department of Nuclear Engineering, 310 Pasqua Engineering Building, Knoxville, TN 37996

Oak Ridge National Laboratory, Nuclear Science and Technology Division, PO BOX 2008, Oak Ridge, TN 37831

INTRODUCTION

Modeling and simulation using Monte Carlo methods is widely used in nuclear reactor criticality benchmarking applications. However, obtaining good statistics not only takes a large amount of computational time, but it has been shown that localized tally uncertainties may be under-predicted by a factor of five or more in select cases[1, 2]. The primary components of this under-prediction include poor sampling due to improper source convergence and cycle-to-cycle correlations in the fission source. Additional components relate to the flux shape and the size of the tally cells. These issues must be understood and dealt with in order to support the practical use of modern Monte Carlo software packages.

COMPUTATIONAL METHODOLOGY

Select pin cell benchmark models taken from Chapter 3 of Reference 3 are modeled using MCNP[1] to examine the various sources of under-prediction. These models feature different axial burnup distributions where the composition of the LWR fuel consists of more reactive, low burnup end regions separated by a long, less active, high burnup region. The flux profiles of these cases, labeled cases 2.1 – 2.3, are provided in Figure 1. One can see that the flux profiles in these models vary considerably along the length of the fuel rod. By performing a rigorous statistical analysis of these cases, the magnitude and behavior of the under-prediction in the uncertainty can be isolated with respect to various Monte Carlo parameters or problem characteristics.

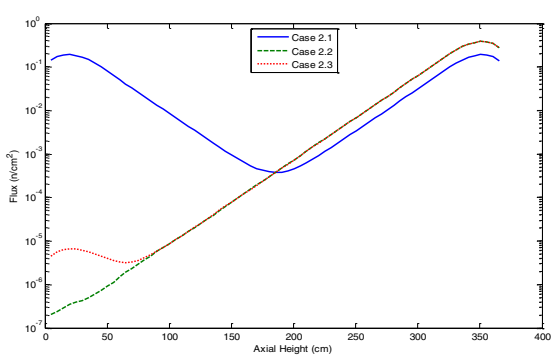

Fig. 1. Flux results for the three benchmark cases

Uncertainty Under-Prediction

To properly identify the under-prediction in the uncertainty, fifty independent simulations were performed for each case in order to obtain true statistical estimates for a particular tally result. The metric used in this analysis is the ratio of the sample standard deviation of the tally mean values for N cases to the average of N standard deviations output by the Monte Carlo code[4]. Different methods were used to examine the sources of under-prediction and their corresponding magnitude and behavior. Investigation of under-prediction due to poor source convergence and sampling involved varying the number of active cycles, number of histories per cycle, and number of initial cycles skipped and observing both k_{eff} and the Shannon entropy as a function of cycle before beginning tally accumulation. Identifying under-prediction due to cycle-to-cycle correlations involved implementing a modified sampling procedure in which the starting source particle distribution was converted into a probability density function along the axial length of the pin cell using the average flux results from previous runs. Then 1,000 cases were run with 100,000 histories per cycle and one active cycle per simulation.

RESULTS

Figure 2 contains results obtained from analyzing axial cell tallies of approximately equal volume for the three benchmark cases. Each case was put through similar analyses to determine the primary component of under-prediction in the uncertainty. By varying the Monte Carlo parameters one can identify whether the under-prediction is a function of poor sampling or cycle-to-cycle correlations.

Case 2.2 shows peak under-prediction in the low-flux regions of the pin cell. By increasing the number of histories per cycle, this factor of under-prediction can be decreased to within reasonable levels. This identifies poor sampling as the primary component of under-prediction. Without enough source sites sampled per cycle, tally uncertainties are under-predicted in the low-flux region of the pin cell.

Case 2.3 is similar to case 2.2, but requires additional skipped cycles to properly converge the fission source because of the small increase in flux near the bottom of the pin cell. The source is converged at approximately 450 cycles, and from Figure 2 one can see that unless

more than 450 cycles have been skipped, the magnitude of under-prediction remains high, and therefore accumulating tallies before the fission source is adequately converged results it under-prediction primarily due to poor sampling. The remaining under-prediction near the bottom of the pin cell can be reduced further by increasing the number of histories per cycle.

Case 2.1 illustrates how large the under-prediction can get when multiple contributing factors are present. Because of the symmetric flux profile, it takes more histories per cycle to adequately converge the source. If the number of active cycles is increased in the presence of a poorly converged source and cycle-to-cycle correlations in the fission source, the uncertainties can be grossly under-predicted, as shown by the initial case. By ensuring that the fission source has been adequately converged and by decreasing the size of the cell tally regions, the factor of under-prediction can be significantly reduced. Note that this particular case is pathologically difficult due to the symmetric flux profile. Since an adequately converged source distribution is more difficult to identify, source convergence still plays a definite role in the magnitude of under-prediction for the final case shown in Figure 2.

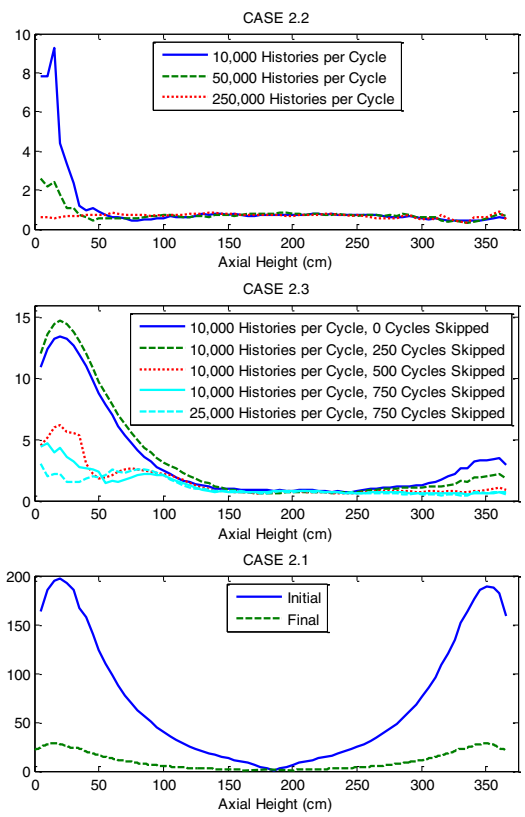

Fig. 2. Comparison of the magnitude of under-prediction in the uncertainty versus axial height for different sets of cases

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