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Godiva IV Thermal Neutron Dosimetry Modeling and Variance Reduction

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Abstract. The transfer of the Godiva IV experiment from the Los Alamos Critical Experiments Facility (LACEF) to the National Critical Experiments Research Center (NCERC) introduced a vastly different experiment room return to the neutron flux. The contribution of the background to the burst neutron energy spectrum is significant in the thermal and epithermal neutron energies. Target materials may be placed in various locations in the Godiva room, or outside of the room, for thermal neutron activation. Modeling of this dosimetry problem in Monte Carlo N-Particle (MCNP) presented a novel challenge compared to previous Godiva IV glory hole irradiation simulations. An advanced dosimetry modeling framework for high efficiency calculations in locations far from the Godiva IV fission source was desired. The mesh-based weight windows and point detector advanced variance reduction techniques in MCNP were implemented and tested using adaptations of the critical experiment benchmark model of the Godiva IV problem. The models were validated against measured activations of Nickel, Indium, Scandium, and Cobalt foils at locations 2 meters from the Godiva IV core. Dosimetry measurements were performed in collaboration with Sandia National Laboratory. The weight windows and point detector variance reduction coupled method resulted in the highest problem efficiency.

1 Introduction

1.1 Motivation

The neutron spectrum of the Godiva IV assembly is being characterized at in-core and ex-core locations to establish the reactor as a known source for neutron dosimetry at the National Criticality Experiment Research Center (NCERC). The Godiva IV fast burst reactor has long been utilized for its high-flux density, fast-neutron environment in the central cavity. Preliminary radiation field characterizations performed at NCERC in the early 2010s showed significant thermalization of neutrons outside of the assembly, attributed to room return. This result was recently confirmed by a Nuclear Criticality Safety Program funded project to characterize the radiation emission of the Godiva IV assembly performed at a number of locations in-core and ex-core. The project was a collaboration between the Sandia National Laboratories' (SNL) Radiation Metrology Laboratory and Los Alamos National Laboratory's NCERC

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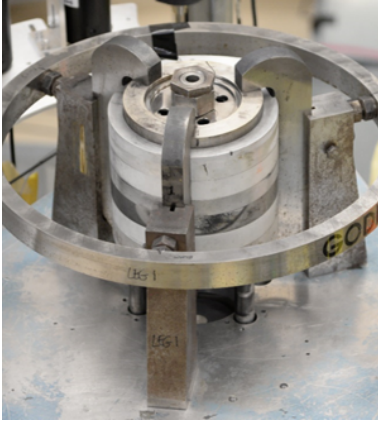
team. Additional dosimetry measurements performed by the NCERC Counting Laboratory (NCERC-CL) (NCERC's in-house reactor dosimetry capability) support the results reported by SNL.

The new dosimetry data generated renewed interest in Godiva IV radiation transport models to simulate the ex-core neutron spectrum at positions of interest for neutron irradiation. The ex-core locations presented a new challenge for simulations not present in the in-core simulations – long run times due to modeling thermalization. We developed a dosimetry modeling framework to provide versatility and efficiency to thermal and epithermal foil activation modeling in Monte Carlo N-Particle (MCNP) code at identified ex-core locations. Variance reduction techniques, such as combinations of the MCNP weight window generator and the F5 tally, were optimized for the Godiva IV problem and its foil locations to improve particle transport to the positions of interest and reduce the runtime for these model results.

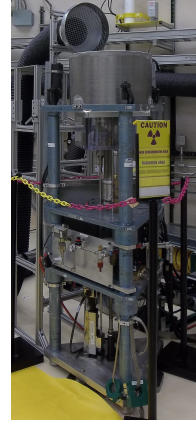
1.2 Godiva IV fast burst reactor

The Godiva IV fast burst reactor assembly, as shown in Figure 1, is composed of six rings, three control rods, and a safety block, each composed of highly enriched uranium (HEU) alloyed with 1.5% molybdenum for strength. The reactor core is mechanically fastened with three clamps and a compression ring. Contamination is minimized with an aluminum “Top Hat” that covers the Godiva IV assembly during operation and a plexiglass box installed underneath (Fig. 1b). The total fuel mass of the system is nominally 65 kg. Originally, the assembly was located in Technical Area 18 (TA-18) at the Los Alamos Criticality Experiments Facility (LACEF). The building that housed the Godiva IV assembly was a sheet-metal structure. This background environment presented a small effect to the radiation field of the assembly. At that time, the Godiva IV assembly had a very well characterized neutron spectrum. A benchmark model was developed for the LACEF configuration of Godiva IV and accepted into the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [1]. With these characteristics, the reactor was a unique source with a reproducible Watt fission energy spectrum.

The Godiva IV reactor assembly was moved from its facility at the Los Alamos National Laboratory to the newly formed National Criticality Experiment Research Center at the Device Assembly Facility in the Nevada National Security Site in 2005. This new environment introduced significant changes from the previous facility at LACEF. At NCERC, the Godiva IV assembly is housed in a smaller, circular concrete experiment facility room, slightly offset from the center of the room. The Comet vertical-lift assembly, another critical experiment at NCERC, is housed in the same experiment facility room, offset from the center of the room in the opposite direction. The many structural elements present have a measurable effect on the spectrum, but the primary contribution to neutron scattering in the room are its thick concrete walls. The perturbed neutron energy spectrum results in measurable differences to the k-eigenvalue of the system as well. The entire room must be modeled to appropriately capture the impact of the thermalized neutrons on the system. This has a large impact on simulation efficiency, particularly for detector response tallies such as reaction rates at ex-core locations.



(a) Assembly with top hat removed.



(b) Full assembly with top hat cover.

Figure 1: Godiva IV fast burst reactor assembly.

2 Methodology

The radiation transport model used for analysis is the revised Godiva IV benchmark MCNP model with the NCERC environment [2]. The Monte Carlo method has allowed for the most accurate depiction of the complex fuel components, shown to inflict significant variation to the overall eigenvalue of the system [2]. The benchmark model is developed to optimize the eigenvalue problem (KCODE).

Since the eigenvalue problem is fundamentally incompatible with advanced variance reduction techniques, a fixed-source model was developed with the benchmark model by adjustment of the control rod positions to make the reactor slightly subcritical. In the fixed source problem, initial spontaneous fission events are sampled proportionally in all fuel cells. The amount of negative reactivity is adjusted to ensure high neutron multiplicity, thereby recovering the neutron spectrum of the critical system.

Select reactor dosimetry foil measurements from the radiation characterization performed by the Sandia National Laboratory Radiation Metrology Laboratory (SNL RML) [3] were used for comparison. From the reported dosimetry locations, the 2 meter location was selected to be the focus of the variance reduction study since it allows for analog simulation for a baseline comparison against variance reduction techniques.

2.1 Variance reduction in Monte Carlo N-Particle

Numerous variance reduction techniques are available in MCNP, and the context of the Godiva IV problem is used to narrow down the list of feasible options (Section 2.7.1.4) [4]. The analog Monte Carlo, and the eigenvalue regime for that matter, both fail to calculate the thermal neutron signature at distance with reasonable efficiency. In the Godiva problem, a thermal neutron can only contribute to a tally on the edge of the room if it scatters many times, reaches thermal equilibrium with the environment, and reaches the tally location. Two variance reduction techniques, the point detector tally and the weight window, introduce different biases to increase the efficiency of this transport problem. [4]

2.1.1 F5, Point Detector Tally

The point detector tally, a partially deterministic method, is a simple variance reduction technique easily configured in a variety of problems. At collision events in the Godiva IV monte-carlo simulation, neutrons are transported using a deterministic estimate to the tally location (Section 2.5.6.1) [4]. The set-up of point detector tallies in the MCNP model is trivial and follows the same formatting as cell flux tallies. The difficulty of point detector tally for the Godiva IV problem stems from reliability concerns with the proper sampling of the large scattering medium of the concrete wall (Section 2.5.6.4.1) [4].

2.1.2 WWG, Weight Window Generator

The weight window technique introduces a bias to the neutron weight as it travels through the phase space of the problem by setting upper and lower weight bounds (Section 2.7.2.12) [4]. Unlike the point detector tally, the weight window is not intended to transport neutrons in the Godiva IV problem to tally locations. It can be employed to give greater importance to regions of space in the Godiva IV geometry. Computer resources are also optimized through the use of Russian roulette for low weight neutrons.

For the Godiva IV model geometry, a cylindrical mesh was used spanning the entire spatial domain as depicted in Figure 2. The green boundary is the concrete wall of the facility, and the entrance is located at the north side. A finer mesh was specified in regions of known interest, such as the Godiva IV assembly and tally location, and a coarser mesh was specified in areas with low expected importance. The weight-window generator was paired with two different types of tallies: F4 and F5.

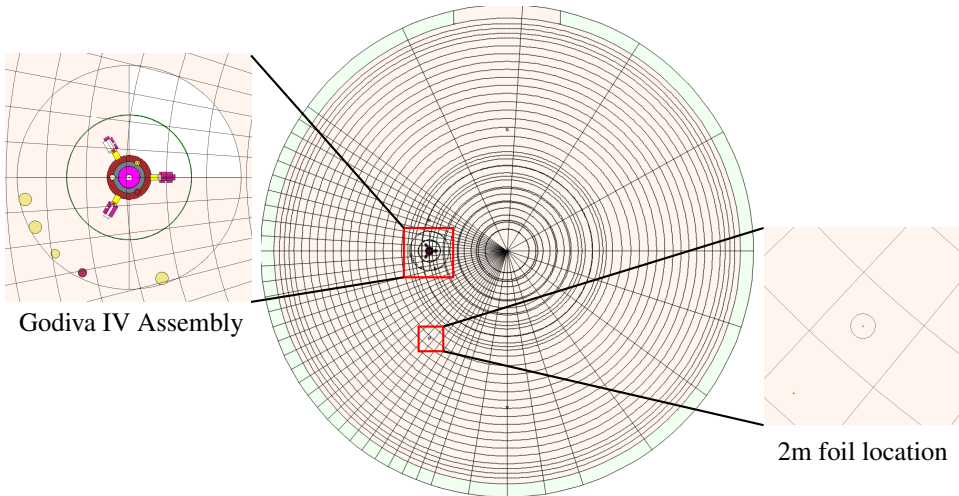


Figure 2: Weight window superimposed mesh on the Godiva model.

2.1.3 F4 Weight Windows

Figure 3 represents the upper weight limits set by the weight window generator in the XY plane for the optimization the neutron energy spectrum at a provided location.

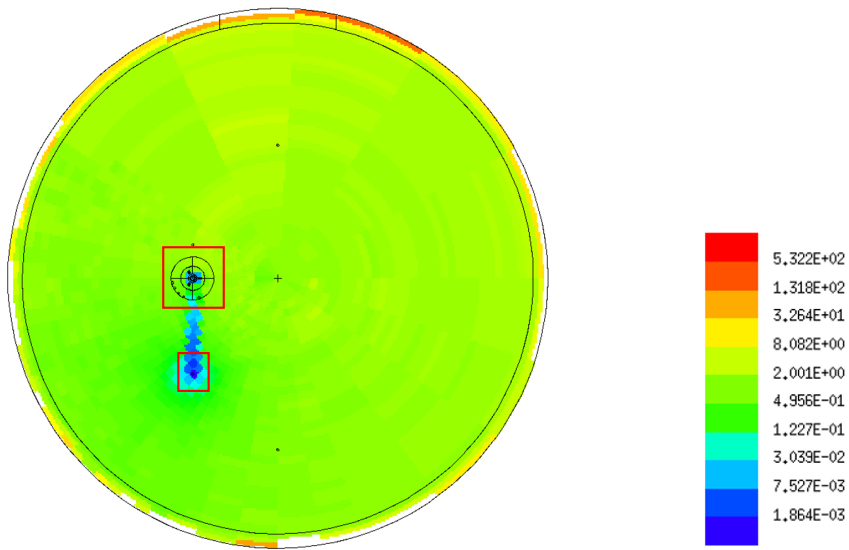


Figure 3: Weight windows in the XY plane for an F4 neutron energy spectrum tally at 2m.

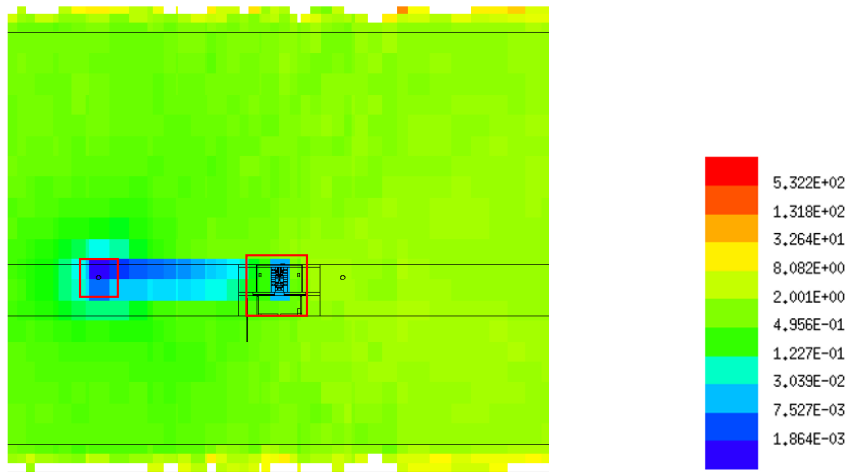


Figure 4: Weight windows in the YZ plane for an F4 neutron energy spectrum tally at 2m.

Similarly, Figure 4 represents the upper weight limits set by the weight window generator in the YZ plane for the optimization the neutron energy spectrum at a provided location.

The weight window generator is a statistic-based algorithm that requires adequate sampling of the space to generate the optimal weight window mesh. The majority of neutrons that contribute to the F4 tally have an initial direction within the solid angle subtended by the tally sphere. This weight window will not increase the efficiency of neutron scattering to the target.

2.1.4 F5 Weight Windows

Figure 5 represents the upper weight limits set by the weight window generator in the XY plane for the optimization the neutron energy spectrum at a provided location. Similarly, Figure 6 represents the upper weight limits set by the weight window generator in the YZ plane for the optimization the neutron energy spectrum at a provided location.

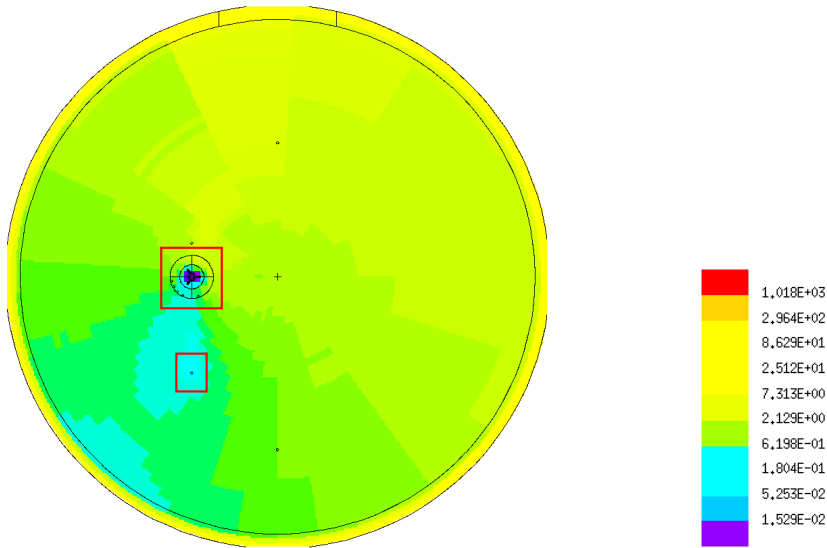


Figure 5: Weight windows in the XY plane for an F5 neutron energy spectrum tally at 2m.

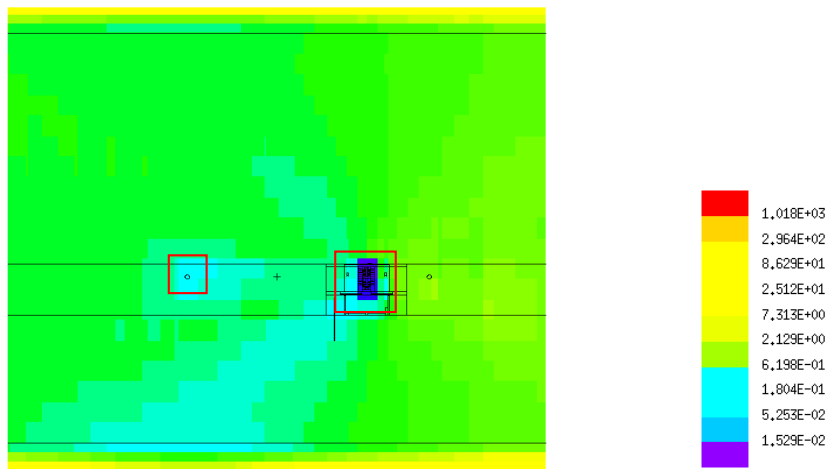


Figure 6: Weight windows in the YZ plane for an F5 neutron energy spectrum tally at 2m.

The weight windows generated for the F5 tally optimization yield a much more favorable outcome compared to the F4 tally optimization. Since the F5 tally is the result of collision based deterministic transport to the provided tally location, neutron scattering contributions

from the concrete wall, floor, and ceiling, are significant. In turn, the forward calculation of the WWG more effectively samples neutron scattering regions, and the weight window parameter output optimizes for these contributions. This approach effectively captures the physics of the problem and increases calculation efficiency for the entire neutron energy spectrum.

3 Results

Each model contained the exact same geometry, and the only perturbation that was performed was the tally type (F4/F5), and the weight-windows (WW). The source was 1×10^7 spontaneous fission neutrons for all simulations. Table 1 contains the simulated reaction rates for the select reactions of interest at the 2 meter dosimetry location.

Table 1: MCNP tally reaction rates for select dosimetry reactions at 2 meters.

Reaction	Tally Type	Reaction Rate	Rel. Error	FOM	Computer Time (min)
$^{58}\text{Ni}(n,p)^{58}\text{Co}$	F4	1.03183E-5	0.0094	0.586	2.1E+04
	F5	1.03952E-5	0.0021	11.5	2.1E+04
	F4 WW	1.04936E-5	0.0115	0.181	4.2E+04
	F5 WW	1.03115E-5	0.0008	308	6.1E+04
$^{115}\text{In}(n,n')^{115m}\text{In}$	F4	2.14465E-5	0.0059	0.586	2.1E+04
	F5	2.16175E-5	0.0021	11.5	2.1E+04
	F4 WW	2.16968E-5	0.0077	0.181	4.2E+04
	F5 WW	2.14444E-5	0.0007	308	6.1E+04
$^{45}\text{Sc}(n,\gamma)^{46}\text{Sc}$	F4	2.20745E-3	0.0057	0.586	2.1E+04
	F5	2.22317E-3	0.0021	11.5	2.1E+04
	F4 WW	2.16414E-3	0.0143	0.181	4.2E+04
	F5 WW	2.20501E-3	0.0008	308	6.1E+04
$^{59}\text{Co}(n,\gamma)^{60}\text{Co}$	F4	3.34298E-3	0.0076	0.586	2.1E+04
	F5	3.37327E-3	0.0021	11.5	2.1E+04
	F4 WW	3.35541E-3	0.0207	0.181	4.2E+04
	F5 WW	3.34440E-3	0.0008	308	6.1E+04

The F5 WW implementation shows the greatest agreement across all four dosimetry reactions with the analog F4 tally result. The standard F5 and F4 WW results across all reactions show that a significant bias is introduced by these two implementations. Between the two, the standard F5 has a smaller bias than the F4 WW implementation.

Tally efficiency in MCNP is described best by the figure of merit (FOM). It is inversely proportional to the computer time and square of the relative error. For each type of tally, the FOM is listed in Table 1. The F5 WW implementation resulted in the largest FOM across all of the techniques, suggesting that the optimized scattering only present in this implementation had a significant role. The standard F4 FOM was greater than the F4 WW FOM, thus the weight window optimization over an F4 tally is shown to hinder the calculation efficiency. The computer time remained the same for standard F4 and F5 tallies, however, the weight window simulations resulted in longer run times for the same source definition. This is attributed to the additional checks the program must perform as neutrons cross mesh-boundaries. Overall, in terms of accuracy and precision, the F5 WW technique provides the most reliable and efficient ex-core simulated reaction rate. Subsequently, the simulated reaction rates were compared to those measured by SNL.

Table 2 contains the measured activity of neutron activation dosimetry and the calculated to experimental (C/E) dosimetry results for the variance reduction implementations.

Table 2: Specific activity C/E values for the variance reduction implementations.

Reaction	Activity (Bq/atom)	C/E-1			
		F4	F5	F4 WW	F5 WW
$^{58}\text{Ni}(n,p)^{58}\text{Co}$ - Ref.	2.0107E-21	0	0	0	0
$^{115}\text{In}(n,n')^{115m}\text{In}$	1.3089E-18	20.99%	21.05%	20.36%	21.06%
$^{45}\text{Sc}(n,\gamma)^{46}\text{Sc}$	1.0078E-19	260.82%	260.70%	247.83%	260.66%
$^{59}\text{Co}(n,\gamma)^{60}\text{Co}$	5.1672E-21	363.76%	364.50%	357.71%	364.26%

The C/E values for the different variance reduction techniques are roughly equivalent, with the notable exception of the F4 WW. The F4 WW, as discussed previously, introduces significant bias to the transport problem as scattering mediums are not efficiently sampled. The large C/E values for the capture reactions, as also reported in SNL's radiation field characterization report, are thus attributed to inaccuracy of the environment modeling in the Godiva IV benchmark.

Preliminary discussion on causes of large calculated to experimental dosimetry results concluded that the actual thermal neutron fluence is significantly lower than the simulated. Thermal neutrons interact with materials very differently from their high energy counterparts, with much higher absorption cross sections. Structures such as the steel rebar in the concrete have not been included in the current benchmark model development. In addition, the major contributor to the thermalization of neutrons in the model is the concrete, and the hydrogen content of the concrete can greatly influence the rate of thermalization. The arid environment at the Nevada National Security Site subjects the concrete structure to greater than average concrete dry-out.

The benchmark Godiva IV model uses Portland concrete as its concrete composition. A substitution was made for the Hanford Dry concrete, which contains the lowest hydrogen atom fraction out of those compiled by Pacific Northwest National Laboratory [5]. Figure 7 quantifies the impact of the concrete composition with respect to hydrogen fraction on the neutron energy spectrum.

The original benchmark k-eigenvalue was evaluated to 1.003161 ± 0.000014 , in a slightly supercritical configuration. The perturbed benchmark k-eigenvalue was evaluated to 1.003124 ± 0.000013 . This represented a negative reactivity insertion of 3.676 pcm.

The variance reduction fixed source implementation was again evaluated with the altered concrete composition. Table 3 contains the measured activity of neutron activation dosimetry, and the calculated to experimental (C/E) dosimetry results for the variance reduction implementations.

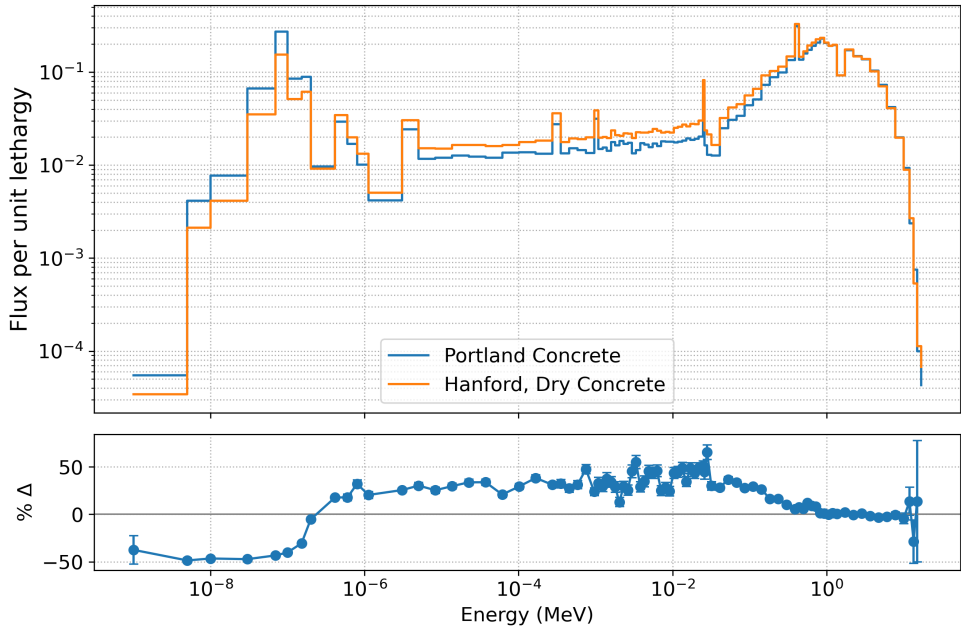


Figure 7: MCNP KCODE Godiva IV benchmark with Hanford Dry Concrete 89-group neutron lethargy fluence energy spectra for the 2m location (logarithmic-logarithmic).

Table 3: Specific activity C/E values for the variance reduction implementations with Hanford Dry Concrete instead of Portland Concrete.

Reaction	Activity (Bq/atom)	C/E-1			
		F4	F5	F4 WW	F5 WW
$^{58}\text{Ni}(n,p)^{58}\text{Co}$ - Ref.	2.0107E-21	0	0	0	0
$^{115}\text{In}(n,n')^{115m}\text{In}$	1.3089E-18	24.34%	23.69%	22.70%	23.74%
		(+3.35%)	(+2.64%)	(+2.34%)	(+2.68%)
$^{45}\text{Sc}(n,\gamma)^{46}\text{Sc}$	1.0078E-19	118.62%	118.15%	109.92%	117.86%
		(-142.2%)	(-142.55%)	(-137.91%)	(-142.8%)
$^{59}\text{Co}(n,\gamma)^{60}\text{Co}$	5.1672E-21	215.32%	214.10%	204.68%	213.73%
		(-148.44%)	(-150.40%)	(-153.03%)	(-150.53%)

As demonstrated by the large reduction in calculated to experimental values for the activation reactions, the lower thermal energy peak is a more accurate depiction of the neutron energy spectrum at 2 meters from Godiva. Further investigation into Godiva IV assembly environment impacts is necessary to determine other significant contributions. Steel rebar in the concrete walls may introduce significant neutron absorption in the walls, not currently modeled. The exact concrete composition is not currently known, but core samples have been extracted and a laboratory analysis will be performed to determine its composition. Lastly, the concrete ceiling thickness may be much less than currently predicted.

4 Conclusion

This investigation demonstrated the effective ease-of-implementation and accuracy of weight windows and F5 point detector tally variance reduction techniques for the Godiva IV system. It was shown that the F5 and weight window combination boosted the sampling of neutron scattering in the Godiva-IV and room system, which was the most effective approach to increasing the figure of merit and overall calculation efficiency. The approach was applied to model the furthest ex-core dosimetry results attained by the Sandia National Laboratories Radiation Metrology Laboratory as reported in the radiation characterization report for Godiva-IV. Good agreement was observed between different modeling techniques, however, sizable calculated to experimental values were determined for the dosimetry reactions. This result aligns with the spectral adjustment performed by SNL. A modification to the concrete composition in the Godiva-IV MCNP model was evaluated yielding improved calculated to experimental results. Future evaluations will take advantage of the increased speed of calculation with variance reduction to continue to test and improve the Godiva-IV model and the simulated spectral accuracy.

5 Acknowledgments

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