Analysis of SCALE Criticality and Sensitivity Calculations for Reflected HEU Cylinders

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ABSTRACT

The SCALE code package offers multiple nuclear data libraries and sensitivity and uncertainty (S/U) methods supporting and derived from Monte Carlo (MC) transport. The CSAS and TSUNAMI-3D sequences use KENO MC, utilizing either continuous-energy (CE) cross sections or multigroup (MG) cross section libraries. TSUNAMI-3D has two CE calculational methods: the iterated fission probability (IFP) method, and the Contribution-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance CHaracterization (CLUTCH) method. Previous work has shown poor agreement between CLUTCH and confirmatory direct perturbation calculations in specific applications (e.g., fissionable and polyethylene reflectors). The HEU-MET-FAST-084 (HMF-084) International Criticality Safety Benchmark Evaluation Project evaluation consists of 27 cylindrical highly enriched uranium metal cores with 14 unique reflector materials of 0.5 and 1 in. thicknesses. Included in this list of reflector materials are natural uranium and polyethylene. This work utilized SCALE 6.2.4 models of the HMF-084 evaluation, with additional non-physical configurations to test both the MG bias and CLUTCH functionality across a variety of reflector material thicknesses. The evaluation's use of concentric cylinders allowed for examination of several MG self-shielding methods: infinite homogenous, cylindrical, and spherical. The results indicate that the use of polyethylene reflectors with CLUTCH is not fundamentally impossible but sensitive to geometry. The poor performance of CLUTCH with fissionable reflectors was reaffirmed. The 2 in. and greater polyethylene-reflected calculations demonstrate the necessity of using the 302-group library for fast systems. The nickel MG bias was substantial, as discussed in a companion paper, as were cobalt and iron.

Key Words: Multigroup, sensitivity uncertainty

1 INTRODUCTION

The SCALE code package offers multiple nuclear data libraries supporting Monte Carlo (MC) transport, with sensitivity and uncertainty (S/U) methods derived from MC transport solutions [1]. The SCALE 6.2.4 MC engine is KENO, which can utilize continuous-energy (CE) cross sections and multigroup (MG) cross sections derived from ENDF/B-VII.1 [2]. Although CE cross sections are not exact and are subject to periodic revisions, they still represent the highest fidelity data. Collapsing energy groups to produce MG cross sections can be done efficiently and accurately, particularly in well studied and popular geometries for improved self-shielding effects. However, this produces a bias, as the cross sections used in calculations are changed. In improving the accuracy and reducing bias, a variety of self-shielding methods have been implemented in SCALE, relating the geometry of the model to spatial effects of self-shielding. Additionally, with neutron energies spanning orders of magnitude, some MG group structures may be inadequate or unintended for a certain application, such as the SCALE 302-group library intended for fast reactors [3]. This study aims to identify MG materials of strong bias in both libraries, as well as establish the conditions at which celldata show optimum performance.

Prior investigation of the KENO-based CE TSUNAMI methods CLUTCH and IFP resulted in unfavorable sensitivities in configurations using specific reflector compositions when taken in reference to confirmatory direct perturbation (DP) sensitivities. Primarily, these have been found in reflector materials that utilize fissionable isotopes (e.g., natural uranium) or polyethylene [4, 5]. Prior investigations have found the poor performance of fissionable reflectors to be related to the number of inactive or discarded generations in the formation of the F* mesh, imposed over fissile material present in the application to determine relative importance functions. However, investigation into polyethylene performance factors was inconclusive. This study with a variety of reflector materials aims to identify the potential of additional reflector materials at odds with the CLUTCH methodology, while confirming prior findings.

2 METHODOLOGY

Models produced for the International Criticality Safety Benchmark Evaluation Project (ICSBEP) benchmark HEU-MET-FAST-084 as part of VALID expansion were used as baseline configurations representing the nominally evaluated conditions [6–9]. Nominal models have reflector thicknesses of 0.5 or 1 in. Only HMF-084-001 through -025 were utilized, as -026 and -027 have two unique concentric reflector materials. Additional model perturbations were created such that each case had variations with reflector thicknesses of 0.5, 1, 2, 4, and 8 in., as shown in Figure 1 (e.g., HMF-084-001 nominally has 1 in. reflector; perturbed new models have 0.5, 2, 4, and 8 in. reflector). These perturbations are meant only as non-physical tests of the CSAS and TSUNAMI methodologies; they do not represent real-life configurations. Each model had a CE calculation, 252-group calculation, and the 302-group calculation taken from a SCALE 6.3 beta. The 1597-group also included in SCALE 6.3 was not investigated as the library file structure is not supported in SCALE 6.2.4. MG calculations were performed with infinite homogenous (inf), cylindrical (cyl), and spherical (sph) self-shielding treatment. These models were run with SCALE 6.2.4 CSAS and TSUNAMI-3D to 0.0001 Δk_{eff} MC uncertainty [1]. CE and infinite homogenous MG inputs required no further manipulation. Cylindrical MG inputs required the multiregion cylindrical radius according to the radius used in the geometry. Spherical MG inputs used volume equivalent radii for each region. These approaches were chosen to achieve a semblance of applicability to the problem of nested cylinders of varying thicknesses—it is expected that with 0.5 in. reflector thickness, for example, infinite homogenous bias would be greater magnitude than the same case with 8 in. thickness and lesser than 0.5 in. with cylindrical or spherical processing. All library and celldata perturbations are presented to demonstrate the effect.

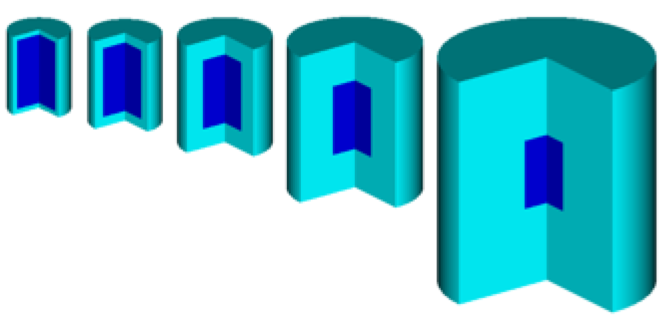

Figure 1. HEU-MET-FAST-084-XXX representative model with variable reflector thicknesses of 0.5, 1, 2, 4, and 8 inches.

Cases were converted to TSUNAMI inputs. This required the revision of the "csas5" identifier to "tsunami-3d-k5". Both the IFP and CLUTCH methods were used, requiring different manipulation. CLUTCH parameters utilized 10 latent generations with a 1 cm mesh. IFP utilized 10 latent generations. These parameters may not be ideal for every given case but were chosen to demonstrate the performance of both methods with the same degree of latent generations, and in the case of CLUTCH, a suitably fine mesh. These parameters are expected to perform well with direct perturbation confirmation in the case of no outstanding nuclear data or geometrical issue.

Cases were run on an ORNL Linux server in parallel with 32 cores. IFP calculations in SCALE 6.2.4 were required to be run serially. Calculated k_{eff} values were pulled from CSAS outputs, and total reflector sensitivity coefficients by mixture from TSUNAMI outputs. The use of total mixture sensitivities may hide more discrete issues within the respective codes, but with 125 cases and a variable number of nuclides per reflector mixture, this broader approach is more directly comparable across all reflector thicknesses, and less tedious. CSAS inputs corresponding to the appropriate TSUNAMI case were reproduced with reflector density perturbations to provide confirmatory direct perturbation calculations for the calculated sensitivities. Deviations between DP and calculated sensitivities were measured as factors of the propagated uncertainties. A discrepancy was noted when this factor reached 2σ, not to mark explicitly as an issue, but to note potential trends. Deviations between CE and MG k_{eff} were relative to CE results, with the difference in k_{eff} noted.

3 RESULTS

3.1 CSAS 252-Group

Calculated k_{eff} values for the CE results were subtracted from 252-group MG k_{eff} such that MG overprediction would be positive. MG bias is presented in Figure 2 as a function of reflector thickness and MG calculated energy of average lethargy of fission (EALF). Apart from a tail beginning around $3x10^5$ eV resulting from polyethylene and beryllium cases -003, -011, -016, and -023, there is no observable trend in bias by EALF, even upon closer inspection of biases at EALF greater than $3x10^5$ eV. There is a clear trend of increasing bias with reflector thickness for all celldata methods. To investigate further, Figure 2 considered the accuracy of the calculated MG EALF, plotting the discrepancy between MG EALF and the CE value against the reflector thickness, resulting in MG underprediction of EALF relative to CE with increased reflector thickness, noticeably similar to the original trend. With this relationship, the MG bias against the relative deviation in EALF between CE and MG values was investigated, showing the MG misprediction in EALF related to bias in k_{eff}.

A summary of biases greater than 500 and 1,000 pcm by reflector material is given in Table I. As noted before, several materials are used twice with both nominal cases summarized by the common reflector material. The arbitrary cutoffs of 500 and 1,000 pcm in bias magnitude were used to highlight materials with poor CE–MG agreement. Biases greater than 1,000 pcm are clearly the more troublesome category: several instances of cobalt, iron, and nickel showed this magnitude. Nickel MG biases are notated separately in a companion paper [10]. The impact of ENDF/B-VIII.0 cobalt revisions was not investigated, which had notable capture changes above 1 MeV and could have since improved with respect to flux estimates for collapse [11]. Not reflected in the table is that all biases greater than 1,000 pcm occur at 8 in., apart from both instances of iron with a 1 in. reflector. Given the trend across all materials, these 8 in. instances of 1,000 pcm bias may be a result of misprediction of EALF, resulting in increased bias rather than specific errors in MG cross sections. However, these materials do have an increased load of 500 pcm or greater for cases even at lower thicknesses. Twenty-six of the 55 instances of bias greater than 500 pcm occur at 8 in. For cobalt, iron, and nickel, eight of the ten infinite homogenous cases have biases greater than 500 pcm. For all three materials, the only instances that do not have bias greater than 500 pcm occur at 4 in. reflector thickness, at a central point between a strong negative bias at 2 in. thickness and strong positive bias at 8 in. thickness. Apart from these three materials, only aluminum and copper reflector have biases greater than 500 pcm. All instances of these occur at 8 in.

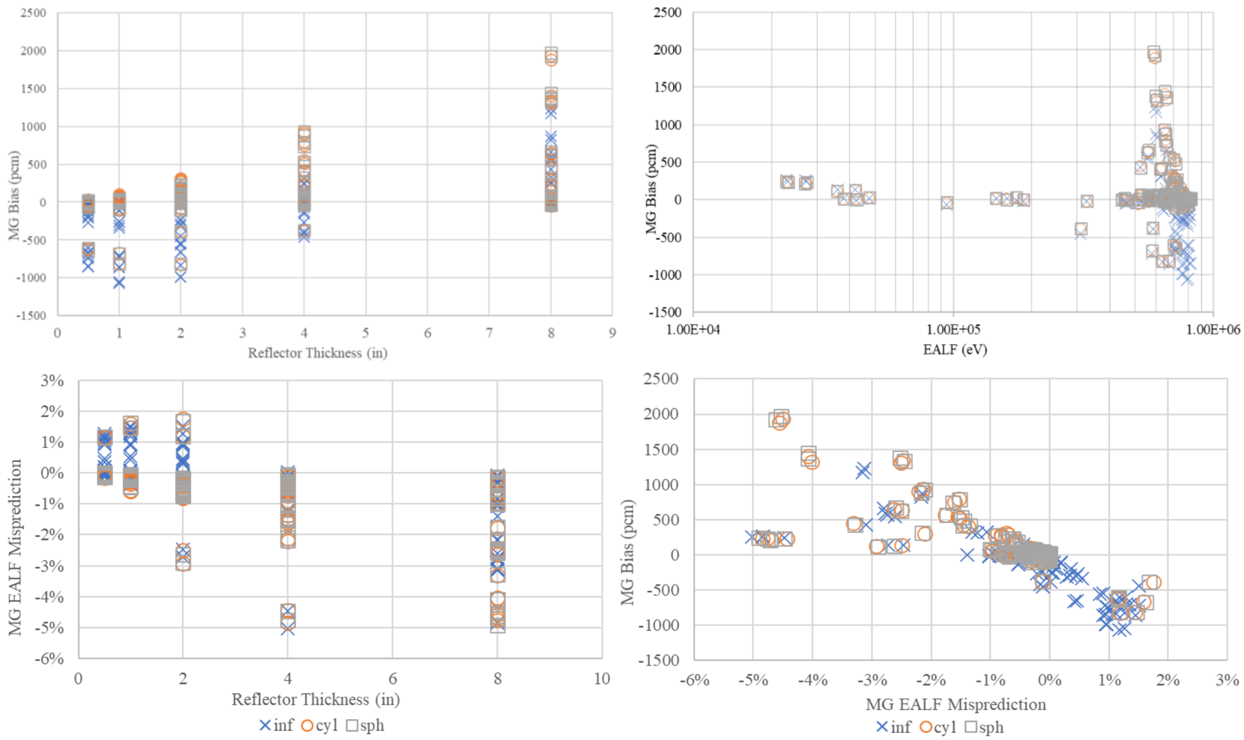

Figure 2. Clockwise from top left for 252-group: MG bias by reflector thickness, MG bias by EALF thickness, MG bias by MG EALF misprediction, MG EALF misprediction by reflector.

Table I. Instances of 252-group bias greater than 500 and 1,000 pcm, by reflector material														
>500	Al	Al_2O_3*	Be*	C	Co*	Cu*	Fe*	Mo*	Mo_2C*	Ni*	Poly*	Ti	U*	W*	Total
Inf	0	0	0	0	8	2	8	0	0	8	0	0	0	0	26
Cyl	1	0	0	0	4	2	4	0	0	4	0	0	0	0	15
Sph	1	0	0	0	4	2	3	0	0	4	0	0	0	0	14
>1000	Al	Al_2O_3*	Be*	C	Co*	Cu*	Fe*	Mo*	Mo_2C*	Ni*	Poly*	Ti	U*	W*	Total
Inf	0	0	0	0	2	0	2	0	0	0	0	0	0	0	4
Cyl	0	0	0	0	2	0	2	0	0	2	0	0	0	0	6
Sph	0	0	0	0	2	0	2	0	0	2	0	0	0	0	6

*Duplicated reflector

Table II (left) displays the average MG bias as a function of celldata and reflector thickness across all cases. Increase in bias with reflector thickness is seen with all celldata apart from an initial drop at 1 in. infinite homogenous. Table II (right) displays the average magnitude of the MG bias as a similar function. Four in. appears as a point of optimum utility for the use of infinite homogenous. Cylindrical and spherical treatments are on average statistically equivalent, with 114 of the 125 cases being within three standard deviations, and all cases within 100 pcm. Below two in., spherical performs the best of all three treatments (though on par with cylindrical). At four and eight in., infinite homogenous performs the best.

Table II. Average and absolute average 252-group bias							
	Inf	Cyl	Sph		Inf	Cyl	Sph
0.5	-226.9	6.5	0.8	0.5	228.8	19.6	16.6
1	-269.3	24.5	10.5	1	274.7	42.1	26.8
2	-202.0	98.0	75.2	2	247.9	113.0	91.0
4	12.7	259.3	252.5	4	129.4	261.9	254.9
8	287.3	471.5	485.0	8	300.9	484.3	494.6

3.2 CSAS 302-Group

The approach for the 302-group calculations was the same as that for the 252-library. MG bias is presented in Figure 3 as a function of reflector thickness and MG calculated EALF. Apart from a tail beginning around 3×10^5 eV resulting from polyethylene and beryllium cases -003, -011, -016, and -023, there is no observable trend in bias by EALF, even upon closer inspection of biases at EALF greater than 3×10^5 eV. This tail illustrates biases up to 8,000 pcm in polyethylene-reflected cases dependent on EALF. The 302-group library is intended for fast systems and therefore does not accurately reflect sufficiently moderated systems. The y-axes of subsequent subfigures in Figure 3 were adjusted after demonstrating the importance of utilizing MG libraries for their intended application. Remaining figures were adjusted to ranges used in Figure 2 of the 252-group for visual comparisons, excluding the thermalized systems with the 302-group library. As before, there is a trend of increasing bias with reflector thickness. However, the range is tighter relative to the 252 group, spanning 1,800 pcm across all cases relative to 3,000 pcm. This ~40% reduction in bias range is also observed at the reflector thickness level, with ranges within a set thickness reducing ~37%—apart from only a 22% reduction for infinite homogenous at 4 in. The EALF misprediction relation to bias is observed again, though with reduced magnitudes on both accounts. A summary of bias by reflector material is given in Table III. As before, cobalt, nickel, and iron stand out as greater than 500 pcm, though of the three materials, only cobalt has bias greater than 1,000 pcm. Polyethylene is above both 500 and 1000 pcm for reflector thickness greater than 2 in. as a result of improper use of the 302-group library. Excluding polyethylene gives rise to biases greater than 1,000 pcm in cobalt alone, with noted improvement in iron and nickel relative to the 252-group. There is also general improvement in using the 302-group library in proper applications

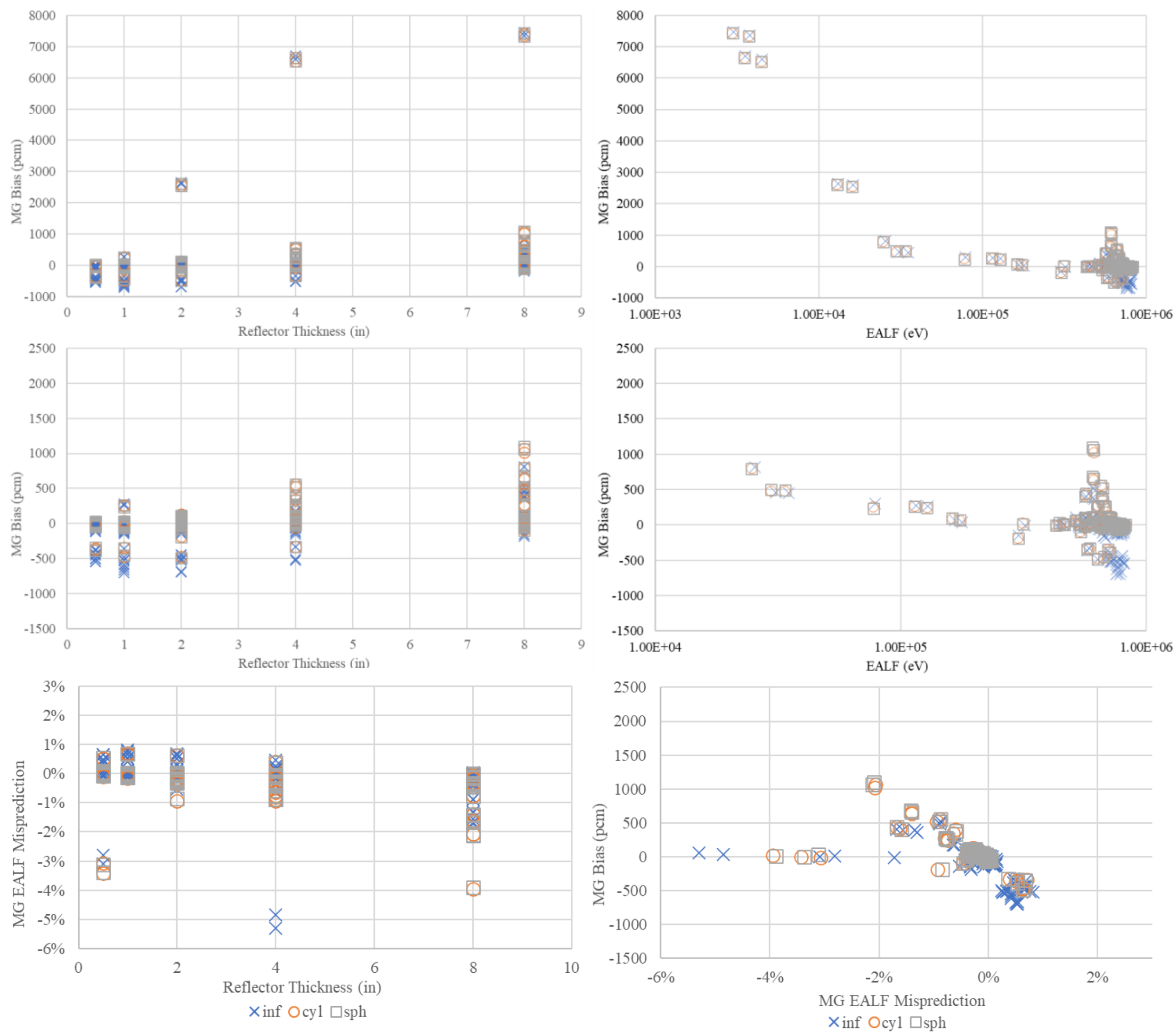

Figure 3. Clockwise from top left for 302-group: MG bias by reflector thickness including polyethylene, MG bias by EALF including polyethylene, MG bias by EALF, MG bias by MG EALF misprediction, MG EALF misprediction by reflector thickness, MG bias by reflector thickness.

Table III. Instances of 302-group bias greater than 500 and 1,000 pcm, by reflector material

>500	Al	Al_2O_3*	Be*	C	Co*	Cu*	Fe*	Mo*	Mo_2C*	Ni*	Poly*	Ti	U*	W*	Total
Inf	0	0	0	0	3	0	8	0	0	6	6	0	0	0	23
Cyl	0	0	0	0	4	0	0	0	0	2	6	0	0	0	12
Sph	0	0	0	0	4	0	0	0	0	2	6	0	0	0	12
>1000	Al	Al_2O_3*	Be*	C	Co*	Cu*	Fe*	Mo*	Mo_2C*	Ni*	Poly*	Ti	U*	W*	Total
Inf	0	0	0	0	0	0	0	0	0	0	6	0	0	0	6
Cyl	0	0	0	0	2	0	0	0	0	0	6	0	0	0	8
Sph	0	0	0	0	2	0	0	0	0	0	6	0	0	0	8

*Duplicated reflector

Table IV (left) displays the average MG bias as a function of celldata and reflector thickness across all cases. Increase in bias with reflector thickness is seen with all celldata apart from an initial drop at 1 in. infinite homogenous. Table IV (right) displays the average magnitude of the MG bias as a similar function. Notably, all approaches show increasing magnitude in bias. However, this includes polyethylene. Table V adjusts for this by removing polyethylene cases, as the 302 library is unsuited for the application. Cylindrical and spherical treatments are on average statistically equivalent, with 120 of the 125 cases being within three standard deviations, and all cases within 60 pcm. As with the 252-group, below two in., spherical and cylindrical perform better than infinite homogenous, whereas at four and eight in., infinite homogenous performs the best.

Table IV. Average and absolute average 302-group bias

	Inf	Cyl	Sph		Inf	Cyl	Sph
0.5	−150.9	−7.5	−9.7	0.5	151.9	12.7	16.9
1	−152.9	23.4	13.9	1	200.3	38.7	37.8
2	68.5	247.7	235.0	2	371.5	256.2	253.1
4	501.3	649.2	645.5	4	638.4	654.5	648.5
8	722.4	826.6	836.8	8	767.4	839.5	846.9

Table V. Average and absolute average 302-group bias, excluding polyethylene

	Inf	Cyl	Sph		Inf	Cyl	Sph
0.5	−164.3	−7.2	−11.5	0.5	164.4	13.0	16.6
1	−189.6	3.1	−6.6	1	194.3	19.8	19.5
2	−153.8	44.9	30.8	2	175.5	54.1	50.5
4	−32.9	132.6	128.9	4	116.1	138.5	132.2
8	140.7	256.7	267.5	8	189.6	270.7	278.5

3.3 CE TSUNAMI

Only three cases greater than 2σ discrepancy were observed between IFP and DP. The maximum is 2.35σ, which is not a concern for agreement. A total of 19 cases greater than 2σ discrepancy were observed between CLUTCH and DP. The maximum is 66.5, though all but six are less than 5σ. Of the cases greater than 2σ, eight are natural uranium reflected, with thickness dependent deviations. Across the 10 cases with natural uranium, fissionable reflector, each doubling of reflector thickness resulted in an approximate tripling of the relative deviation between DP and CLUTCH (i.e., deviations of 1.1, 2.5, 7.4, 24.0, and 66.5σ at the investigated thicknesses). At the greatest reflector thickness investigated, the relative deviation as a percent was ~45% in both cases. This provides supplementary evidence of CLUTCH failing to accurately calculate sensitivities in situations with fissionable reflectors [4]. Attempts to reduce the deviation were not attempted again as previously reported, as previous reporting already noted that the use of increased inactive generations reduced the deviation at great computational expense. Future investigation could elucidate potential trends of the required number of discarded generations with reflector thickness.

Four of the 19 cases greater than 2σ are polyethylene reflected. The maximum is 3.49σ, but an absolute difference in sensitivity of 0.005 %Δk/%ΔΣ. Although the deviations are not concerning themselves, that only the 0.5 and 1 in. cases have this magnitude of deviation suggests that thin layers of polyethylene are more sensitive to the CLUTCH method. Compared with results from Marshall et al., the most similar case examined was PMF-024 which did not detail CLUTCH meshing or latent generations in text, but upon private communication with the authors, was determined to be comparable to the approach in this study [5, 12, 14]. The 1.55 cm (0.61 in.) spherical shell of polyethylene resulting in a DP CLUTCH deviation of 4.3σ is not substantially different from the 3.49σ observed at 0.5 in. [5]. PMM-002 cases utilized interspersed and frame polyethylene no thicker than 1 in., potentially agreeing with the possibility that geometrical effects are key to the observed DP deviations greater than 10σ [13].

4 CONCLUSIONS

This study was performed to investigate the SCALE KENO MC engine across KENO-derived sequences CSAS and TSUNAMI, investigating MG library biases and sensitivity calculational methods across nonphysical configurations. Prior and ongoing work found inaccuracies in both sequences, which was further investigated utilizing the HEU-MET-FAST-084 ICSBEP critical benchmark, chosen for its geometrical simplicity and abundance of reflector materials. The perturbation of the reflector thickness across the various reflector materials allowed for an assortment of materials to be tested swiftly and in a uniform approach for each sequence and method. The major points of investigation were 252-group criticality calculations with CSAS, 302-group criticality calculations with CSAS, and CE sensitivity calculations with TSUNAMI CLUTCH.

In perturbing the reflector thicknesses of HMF-084, the most apparent observation was an increasing bias of the 252-group k_{eff} relative to the CE result, in both direction and magnitude. Upon further investigation, the bias was related to a decreasing MG estimate of the energy of the average lethargy of fission, again relative to the CE estimate. Reflector materials of significant bias included cobalt, nickel, and iron, demonstrating in several cases biases greater than 1,000 pcm, and additional cases demonstrating more consistent biases greater than 500 pcm. These biases were most prominent in the use of infinite homogenous celldata processing for self-shielding effects, and at reflector thicknesses of 4 in. or greater. As expected, increased thickness showed better agreement for infinite homogenous cases than the use of cylindrical or spherical celldata, with the inverse true for 2 in. and less. A balance between inadequate infinite homogenous modeling of thin reflector and the MG biasing with thickness was reached, resulting in improved agreement at 4 in. with infinite homogenous celldata.

Repeating the calculations with the 302-group library, the most apparent observation was the extreme outlier in polyethylene reflector 2 in. or greater. This was a known potential result of using the 302-group library, as it is structured and intended for fast system applications. With sufficient polyethylene to moderate neutrons, the structure was no longer appropriate for the system, resulting in biases nearing 8,000 pcm and serving as a demonstration to use MG libraries according to their intended use. Excluding polyethylene, a similar trend was present with the 302-group library, with increasing bias in both direction and magnitude. Again, the bias was related to a decreasing MG estimate of the energy of the average lethargy of fission. With the 302-group library, only cobalt and polyethylene presented biases greater than 1,000 pcm. Removing polyethylene in both sets for consistency, the 302-group showed approximately a 40% reduction in the average magnitude of bias across all celldata and thicknesses. For infinite homogeneous, this was an average of a 30% reduction across all thicknesses, a near 50% reduction for cylindrical celldata, and 45% for spherical. Again, increased thickness showed better agreement for infinite homogenous cases than the use of cylindrical or spherical celldata, with the inverse true for 2 in. and less. A balance between inadequate infinite homogenous modeling of thin reflector and the MG biasing with thickness was shown again, resulting in improved agreement at 4 in. with infinite homogenous celldata.

Finally, upon investigating the IFP and CLUTCH TSUNAMI methodologies, at an equal number of latent generations, IFP produced extremely reliable results, with 3 of 125 cases producing a 2σ discrepancy between IFP and DP. Although 85% of CLUTCH sensitivities were within 2σ as well, notable issues arose with fissionable natural uranium reflector, as anticipated. Errors in DP CLUTCH agreement of up to 45% were observed, with error increasing with reflector thickness, as previously exhibited. In reference to other previous findings, however, polyethylene was unexpectedly tame. Errors in DP CLUTCH agreement remained below 3.5σ, with acceptable absolute deviations. Observed errors were prejudicially present in cases with low reflector thickness, agreeing with previously observed findings while suggesting that thin layers of polyethylene may be key to the observed prior issue, and polyethylene in CLUTCH calculations.

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