DETERMINISTIC–MONTE CARLO HYBRID METHODS FOR EIGENVALUE SENSITIVITY COEFFICIENT CALCULATIONS

T. M. Greene [(1)] *, K. Bekar[(1)], and W. J. Marshall [(1)]

[(1)] *Oak Ridge National Laboratory, 1 Bethel Valley Road, Oak Ridge, Tennessee, 37831, USA*
** greenetm@ornl.gov*

ABSTRACT

The TSUNAMI suite within the SCALE code package includes several methods for generating sensitivity data, including multigroup (MG) and continuous-energy (CE) capabilities. For generating sensitivities with CE data, three methods are available in SCALE 6.3.0: (1) the iterated fission probability (IFP) method with the KENO Monte Carlo transport solver, (2) IFP with the Shift Monte Carlo transport solver, and (3) the Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance Characterization (CLUTCH) with the KENO Monte Carlo transport solver. Currently, it is difficult to generate accurate sensitivities with large reflectors when using the CLUTCH method, specifically with fissionable and hydrogenous materials. To address this issue, the work presented herein examines a methodology to calculate the adjoint flux externally with the 3D deterministic S_N *transport code DENOVO in SCALE; the result is then read directly into the CLUTCH-TSUNAMI sequence. This hybridization method replaces the Monte Carlo* $F^*(r)$ *calculation in CLUTCH while still utilizing the forward calculation. The critical benchmark HEU-MET-FAST-028-001 is used to generate sensitivities based on the inability of CLUTCH to generate accurate sensitivities. Results from the hybrid method appear to generate sensitivity values that are in excellent agreement with direct perturbations. Although further testing is needed, the method provides promising results for the development and utility of a hybrid method for use in TSUNAMI.*

KEYWORDS

Hybrid, sensitivity, CLUTCH

1. INTRODUCTION

The SCALE 6.3.0 code package contains three methods for determining the sensitivity of k_{eff} to each nuclide reaction–specific cross section in the TSUNAMI-3D sequence: (1) a multigroup (MG) approach, which calculates sensitivity coefficients through the use of tallying the forward and adjoint fluxes in a system as a function of space, energy, and angle; (2) the iterated fission probability (IFP) method, which uses continuous-energy (CE) cross sections and determines the importance of events by examining the population of neutrons in the system that are descendants of the neutron that initiated the event; and (3) the Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance CHaracterization (CLUTCH) method, which also uses CE cross sections and calculates the importance of events during a particle's lifetime by examining how many fission neutrons are created by a particle after those events occur. All TSUNAMI-3D sequences are available with the KENO Monte Carlo transport code, whereas only the IFP method is available with the Shift Monte Carlo transport code [1].

The MG sequence calculates sensitivity coefficients using the adjoint-based perturbation theory approach, which calculates both the forward and adjoint flux. CE calculations, however, do not explicitly calculate the adjoint flux and instead rely on different methods to determine a neutron's importance when calculating the sensitivity of k_{eff} to cross section perturbations. Specifically with CLUTCH, the method calculates sensitivities based on Contributon theory [2], which determines the importance of a neutron at a collision by creating and simulating secondary particles at the site of the collision by examining the random walks of forward neutrons.

To calculate the importance of neutrons, the current implementation of CLUTCH uses the IFP method to estimate the F*(r) weighting function, which is the expected importance generated by a fission neutron emitted. This calculation for CLUTCH occurs during the inactive or skipped generations. Currently, the CLUTCH method is known to have difficulties in generating accurate sensitivities for systems with large reflectors, specifically with fissionable (e.g., natural uranium) and hydrogenous materials (i.e., water and polyethylene [3, 4]). For these issues, it has been observed that the F*(r) mesh associated with the model sometimes has convergence issues, which may affect the accuracy of the sensitivity calculations for some systems. To address this issue, the work presented here introduces a novel approach to estimate F*(r) more accurately using the deterministic transport solution for the system. To calculate sensitivities with this new approach, the TSUNAMI sequence in SCALE reads in an externally calculated F*(r) function and uses it with the CLUTCH method to generate sensitivity coefficients.

The critical benchmark HEU-MET-FAST-028-001 (HMF-028-001), Flattop [5], was selected for demonstration and testing applications for the new method based on the expectation for improved results. This experiment is a highly enriched uranium (HEU) sphere reflected by a natural uranium reflector and based on the previous work by Marshall et al. [3], the CLUTCH methodology has difficulties generating accurate sensitivities for ^{238}U in the reflector region.

2. METHODOLOGY

To understand how the $F^*(r)$ function operates, it is useful to step back for a moment and examine how the CLUTCH method simulates neutron importance. Generally, the CLUTCH method calculates sensitivities based on the Contributon theory developed by Mark Williams, which determines the importance of a neutron at a collision site by creating and simulating secondary particles at the point of collision by examining the subsequent random walks of associated forward neutrons [2]. The neutron importance is thus calculated with Eq. (1):

$$\boldsymbol{\phi}^*(\boldsymbol{\tau_S}) = \frac{\lambda}{Q_S}\int_V G(\tau_S \rightarrow r)F^*(r)dr, \tag{1}$$

where $\boldsymbol{\phi}^*(\boldsymbol{\tau_S})$ is the neutron importance in phase space τ_S; Q_S is the fission source in phase space; G $(\tau_S \rightarrow r)$ represents the expected number of fission neutrons generated in all energies and directions from a source neutron at τ_S; and $F^*(r)$ is the expected importance generated by fission neutrons. $G(\tau_S \rightarrow r)$ can be represented with Eq. (2):

$$G(\tau_S \rightarrow r) = \frac{1}{Q_S(\tau_S)}\int_E \int_\Omega \nu\Sigma_f(e,E)\phi(r,E,\Omega|Q_S(\tau_S))d\Omega dE, \tag{2}$$

where $\phi(r,E,\Omega|Q_S(\tau_S))$ is the forward flux generated in phase space (r,E,Ω) from fission source $Q_S(\tau_S)$, and $F^*(r)$ can be represented with Eq. (3):

$$F^*(r) = \int_E \int_\Omega \frac{\chi(r,E)}{4\pi}\phi^*(r,E,\Omega)\, d\Omega dE, \tag{3}$$

where $\chi(r,E)$ is the fission spectrum, and $\phi^{*}(r,E,\Omega)$ is the adjoint flux [1].

In practice, the CLUTCH method calculates the integral of $G(\tau_S \rightarrow r)$, weighted by $F^{*}(r)$, to estimate the importance of every event in a particle's lifetime. In the existing CLUTCH framework, the F*(r) function is estimated from the unconstrained fission spectrum sensitivity coefficient, which is calculated by the IFP approach during the inactive or skipped generations of the Monte Carlo simulations. In contrast, the new hybrid methodology directly calculates F*(r) using an adjoint flux solution from a deterministic solver and the neutron birth spectrum ($\chi(r,E)$) in each mesh voxel.

When testing the validity of the new hybrid F*(r) calculation capability, the only code modification made to the TSUNAMI sequence was adding a capability that enables loading the F*(r) data from an external mesh file (*3dmap* file). The process for generating sensitivity coefficients with the new hybrid method involves several steps. First, a fission source map is generated using the CSAS5 sequence in SCALE 6.3.0 with the Shift Monte Carlo transport code based on a specified uniform mesh grid [1]. This distribution is saved into the Shift *h5* output file. The Shift fission source, along with the mesh grid information, is then read into a DENOVO calculation. DENOVO then performs a source adjoint calculation, using the composition and geometry information from the CSAS5 model, to generate the adjoint fluxes that are saved to the DENOVO *h5* output. Fig. 1 presents a rendering of the total adjoint flux from DENOVO.

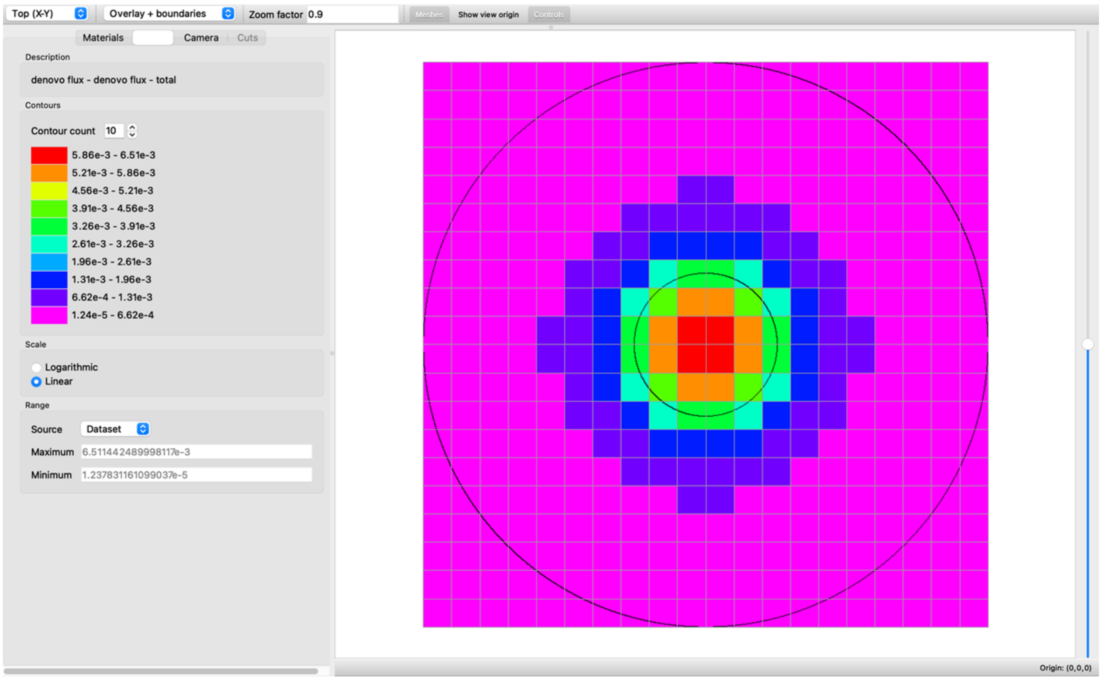

Figure 1. Adjoint flux from DENOVO

However, an additional piece of information is missing from Fig. 1. This is the $\chi(r,E)$ distribution associated with the adjoint flux that is used to calculate the F*(r) function. An additional CSAS5 calculation with KENO V.a [1] was used to estimate χ for the model. This information is referred to as the *birth spectrum*. Once the F*(r) function has been calculated by using both pieces of information, the TSUNAMI-3D sequence is utilized with the CLUTCH methodology to generate sensitivity coefficients.

The hybrid methodology described above was tested with a 20×20×20 uniform mesh along with two different multigroup libraries for the adjoint calculation testing purposes. Additional sensitivity calculations were performed using (1) TSUNAMI-1D–the multigroup deterministic method that uses the transport code XSDRN, (2) TSUNAMI-3D with the MG method, (3) TSUNAMI-3D IFP, and (4) the current TSUNAMI-3D CLUTCH implementation [1]. The two MG libraries were used for the fission source, birth spectrum, and adjoint flux calculations. The 252-group library was also used for the MG and 1D sensitivity calculations. The ENDF/B-VII.1 CE library was used for the hybrid, CLUTCH, and IFP calculations [6]. These results were then compared with the existing sensitivity methods available in SCALE 6.3.0: CLUTCH, IFP, MG, and TSUNAMI-1D. Additionally, the CLUTCH and MG methods also utilized the 20×20×20 uniform mesh for comparison purposes.

All hybrid inputs utilized 10,000 neutrons per generation with the ENDF/B-VII.1 252-group and 1597-group libraries [6]. To demonstrate the effectiveness of the new hybrid method, multiple calculations with 6, 100, and 1,000 skipped generations (parameter *nsk*), respectively, were performed. The CLUTCH inputs utilized 10,000 neutrons per generation while skipping the first 1,000 generations for the F^*(r) calculation. The IFP and MG-forward calculations utilized 10,000 neutrons per generation while skipping the first 100 generations, whereas the MG-adjoint calculation utilized 150,000 neutrons per generation after skipping the first 300 and run to an uncertainty of 100 pcm. All CE calculations—IFP, CLUTCH, and hybrid—utilized five latent generations. The Monte Carlo calculations were run to a k_{eff} uncertainty of 10 pcm, and generated sensitivities were confirmed with direct perturbations (DPs) to support the validity of the calculated sensitivities. The DENOVO adjoint flux calculations used a zero scattering order and a level-symmetric quadrature set of order 16 for testing purposes.

3. RESULTS

Table I presents the results of the TSUNAMI sensitivity calculations with the different methods along with the corresponding DPs. Only two nuclides were identified in the system for analysis: ^{235}U in the central core sphere and ^{238}U in the natural uranium reflector. These preliminary results indicate that the hybrid-generated sensitivities agree very well with the DPs as well as the IFP, 1D, and MG calculations. Compared directly with CLUTCH, the hybrid method appears to accurately generate sensitivities using the same $F^*(r)$ function.

In general, the ORNL guidance for evaluating TSUNAMI sensitivities with DPs is to have differences less than 5%, less than 2σ, and less than 0.0100 [7]. As can be observed in Table I in the highlighted values, the CLUTCH method fails to meet the thresholds for all three categories for ^{238}U. However, by using the external adjoint flux and birth spectrum, the hybrid-generated sensitivities are in very good agreement with the DP generated results. There also is very little difference in the calculated sensitivities from the hybrid method using different numbers of skipped generations. This is a result of the external F^*(r) calculation, which is independent of the number of skipped generations. The hybrid sensitivities also increase in agreement as the number of energy groups in the MG library used for the deterministic adjoint flux increase from 252-groups to 1597-groups. This result is not surprising given the increased refinement of the cross sections used for calculations.

Fig. 2 presents the F^*(r) meshes for the normal CLUTCH method and Fig. 3 for the hybrid method, each with the 20×20×20 uniform mesh and the 252-group library. The externally supplied F^*(r) function more accurately represents the system than the simulated adjoint values from the normal F^*(r) calculation. Each mesh voxel in the hybrid model provides the necessary adjoint flux and birth spectrum information, whereas the CLUTCH method has multiple voxels with no importance information in the reflector region. As noted in [3], at least 10,000 skipped generations are needed in the normal CLUTCH method to provide comparable sensitivities to the other methods. The hybrid method thus appears to have the ability to provide more accurate calculations with less computational time (i.e., skipped generations).

Table I. Sensitivity results

Method	Nuclide	TSUNAMI results		DP results		Results comparison		
		S	σ_S	S	σ_S	% diff.	σ diff.	ΔS
1D	^{235}U	0.5847	--	0.5827	--	0.35	--	0.0020
	^{238}U	0.2082	--	0.2056	--	1.26	--	0.0026
MG	^{235}U	0.5823	0.0013	0.5889	0.0036	-1.11	1.69	-0.0065
	^{238}U	0.2059	0.0011	0.2073	0.0014	-0.67	0.76	-0.0014
IFP	^{235}U	0.5857	0.0006	0.5893	0.0058	-0.61	0.62	-0.0036
	^{238}U	0.2081	0.0006	0.2117	0.0029	-1.72	1.23	-0.0036
CLUTCH	^{235}U	0.5798	0.0002	0.5893	0.0058	-1.60	1.63	-0.0094
	^{238}U	0.1993	0.0003	0.2117	0.0029	-5.90	4.26	-0.0125
Hybrid	20×20×20	nsk=6						
252-group	^{235}U	0.5966	0.0002	0.5893	0.0058	1.24	1.27	0.0073
	^{238}U	0.2174	0.0003	0.2117	0.0029	2.66	1.92	0.0056
1597-group	^{235}U	0.5947	0.0002	0.5893	0.0058	0.92	0.94	0.0054
	^{238}U	0.2163	0.0003	0.2117	0.0029	2.17	1.57	0.0046
Hybrid	20×20×20	nsk=100						
252-group	^{235}U	0.5965	0.0002	0.5893	0.0058	1.22	1.25	0.0072
	^{238}U	0.2169	0.0003	0.2117	0.0029	2.44	1.76	0.0052
1597-group	^{235}U	0.5946	0.0002	0.5893	0.0058	0.91	0.92	0.0053
	^{238}U	0.2159	0.0003	0.2117	0.0029	1.96	1.41	0.0041
Hybrid	20×20×20	nsk=1000						
252-group	^{235}U	0.5965	0.0002	0.5893	0.0058	1.22	1.25	0.0072
	^{238}U	0.2168	0.0003	0.2117	0.0029	2.37	1.71	0.0050
1597-group	^{235}U	0.5963	0.0002	0.5893	0.0058	1.19	1.21	0.0053
	^{238}U	0.2157	0.0003	0.2117	0.0029	2.37	1.71	0.0040

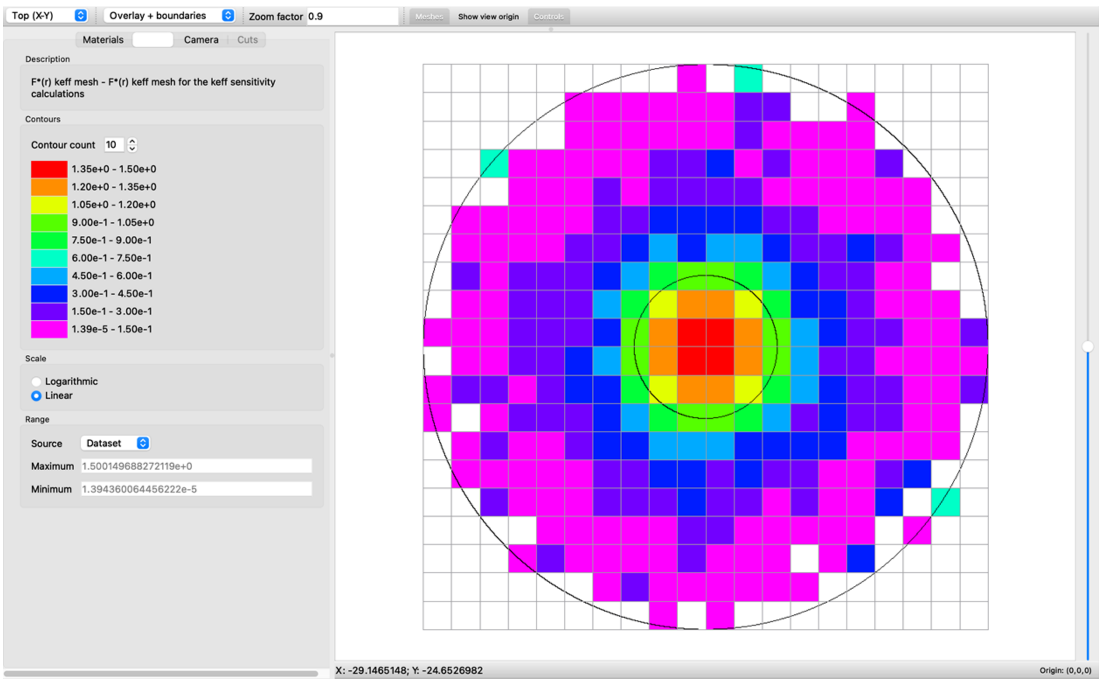

Figure 2. *F(r) mesh for CLUTCH method with 20×20×20 uniform mesh and the 252-group library**

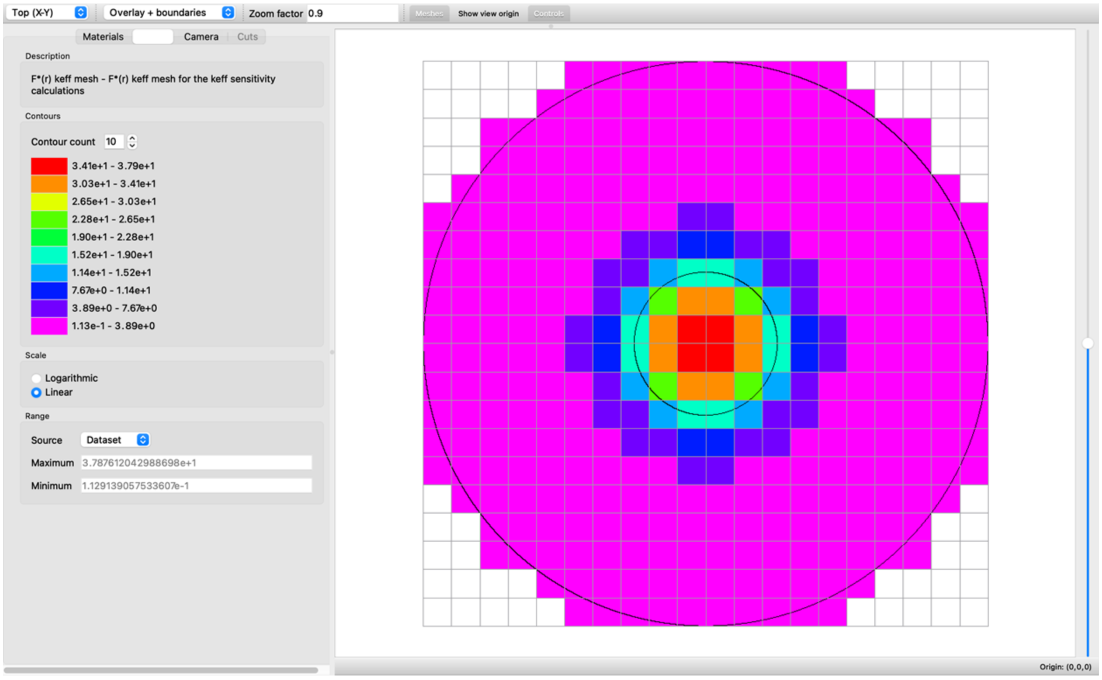

Figure 3. ***F****(r)* **mesh for hybrid method with 20×20×20 uniform mesh and the 252-group library**

As noted above, with the normal CLUTCH calculation, more neutrons and/or more generations would be needed to sample each voxel so as to generate enough information to represent the adjoint flux more accurately and lower the uncertainty of the *F**(r) function. Since the hybrid method already supplies an exact solution for the adjoint flux for each voxel with the associated χ values, the *F**(r) function can be used to generate sensitivities that are more representative of the system as confirmed with the DP results. As an additional comparison, the total sensitivity profiles for ^{238}U in the reflector region are presented in Fig. 4, with the 252-group adjoint flux for the hybrid value.

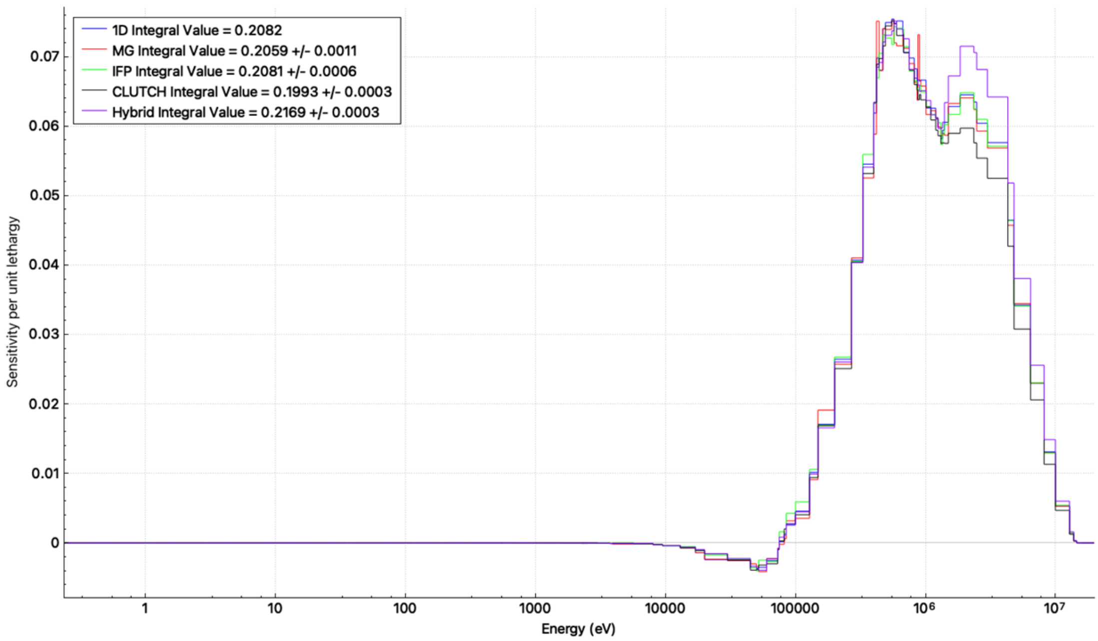

Figure 4: ^{238}U total sensitivity in the reflector region

In general, all sensivitiy calculations from each TSUNAMI method are in good agreement; however, there is a noticeable difference that occurs in a spike just past 1 MeV that is the cause of the differences between the CLUTCH and hybrid methods when compared to the others. From the sensitivity plots it can be observed that the CLUTCH method is underpredicting the sensitivity in ^{238}U, whereas the hybrid method for both MG libraries appears to overpredict it. The cause of the underprediction in CLUTCH can be attributed to the under-sampling of mesh voxels in the system. The cause of the overprediction of the hybrid method requires further investigation. It could be that the chosen parameters for the adjoint calculation are causing this spike in the upper energy region of the sensitivity profile. Additional calculations with higher scattering orders, different quadrature sets, and/or varying mesh grids are needed and may help to explain this further.

4. CONCLUSIONS

The basis for the hybrid sensitivity method came from a need to find a way for CLUTCH to generate sensitivities more accurately for systems with large reflectors of fissionable or hydrogenous material. This approach was demonstrated with the critical benchmark HMF-028-001, Flattop, based on previous work detailing CLUTCH's inability to generate accurate ^{238}U sensitivities within the large natural uranium reflector [3]. The method uses a novel approach to generate sensitivity coefficients by calculating the $F^*(r)$ function externally, which can be read directly in the TSUNAMI sequence. With the importance of each voxel predetermined with the adjoint flux, the hybrid method can more accurately generate the correct sensitivity value for ^{238}U in the reflector region, which is confirmed by the very good agreement with the DP value. Although more testing is needed for other types of systems and materials (i.e., thermal and intermediate systems with different moderators and reflectors), the initial results are very promising for the continued development of the hybrid sensitivity method.

ACKNOWLEDGMENTS

This work was supported by the Nuclear Criticality Safety Program, which is funded and managed by the National Nuclear Security Administration for the US Department of Energy.

REFERENCES

[1] Wieselquist, W. A. and Lefebvre, R. A. (Eds.), SCALE 6.3.0 Manual, ORNL/TM-SCALE-6.3.0, 2021.

[2] Williams, M. L., "Generalized Contributon Response Theory," *Nuc. Sci. Eng.*, 1991, Vol. 108, 4, p. 355-383.

[3] Marshall, W. J., Clarity J. B., and Saylor, E. M., "Sensitivity Calculations for Systems with Fissionable Reflector Materials Using TSUNAMI," *Trans. Am. Nucl. Soc.*, 2018, Vol. 19, 1, p. 787-790.

[4] Marshall, W. J. and Lang, A., "Sensitivity Calculations for Systems with Polyethylene Reflector Materials Using CLUTCH," *Trans. Am. Nucl. Soc.*, 2021, Vol. 124, 1, p. 376-378.

[5] *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, NEA/NSC/DOC(95)03, Organisation for Economic Co-operation and Development, Nuclear Energy Agency, Paris, France (2022).

[6] Chadwick, M. B. et al., "ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data," *Nucl. Data Sheets*, 2011, Vol. 112, p. 2887-2996.

[7] Marshall, W. J. and Rearden, B. T., "The SCALE Verified, Archived Library of Inputs and Data – VALID," *Proceedings of the ANS Nuclear Criticality Safety Division Topical Meeting (NCSD2013)*, 2013.