Sensitivity Calculations for Systems with Fissionable Reflector Materials Using TSUNAMI*

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INTRODUCTION

The SCALE 6.2.2 code package [1] contains four sequences for calculating k_{eff} sensitivity coefficients. Two of these sequences use deterministic transport solvers: a one-dimensional (1D) capability based on XSDRN and a two-dimensional (2D) capability based on NEWT. These sequences are restricted to the multigroup (MG) treatment of neutron energy. The three-dimensional (3D) sequences use the KENO V.a or KENO-VI Monte Carlo transport codes and can be used to calculate sensitivity coefficients with either MG or continuous-energy (CE) transport. The 3D sensitivities are ultimately reported in a MG structure, regardless of the method used in the transport calculations. If desired, the sensitivity coefficients can be reported with very fine energy resolution from a CE calculation, but they are limited to 252 energy groups in the MG mode. CE TSUNAMI methods are available in SCALE starting in SCALE 6.2 [2]. Sensitivity coefficients are generated using the 3D sequences as part of the generation of the SCALE 6.2.2 Validation Report [3]; some difficulties encountered when using the CLUTCH method are discussed and investigated in this paper.

The VALID library maintained at Oak Ridge National Laboratory [4] contains reviewed models of over 600 critical experiment configurations, with TSUNAMI-3D models for over 400. The majority of the ^{233}U critical experiments do not have TSUNAMI models in VALID at this writing. Based on prior work evaluating CE and MG TSUNAMI-3D [5], MG TSUNAMI was used for thermal-spectrum systems, and CE TSUNAMI was used for fast-spectrum systems. This decision was based on the figure of merit (FOM) for the highest uncertainty isotope in the models. The CLUTCH method was chosen over the iterated fission probability (IFP) method within CE TSUNAMI because (1) it generally has a higher FOM, and (2) it has been implemented in parallel within SCALE 6.2.2. Executing CLUTCH in parallel allows calculations to be performed in reasonable time periods.

Direct perturbation (DP) calculations [6] were performed for models which used CE TSUNAMI for the first time. These calculations allow confirmation that the total sensitivity coefficient is correct for important isotopes with large sensitivities in the system. Discrepancies were detected for CLUTCH-calculated sensitivity coefficients in the reflector of a critical experiment if the reflector contained a fissionable material. In most cases, these reflectors were natural or depleted uranium, but in one case a thorium reflector was used. A simple study was performed with spherical systems to further investigate this phenomenon, the results of which are presented here, along with a summary of results for other systems in the VALID library. The results of this study indicate that CLUTCH results should be confirmed by DP calculations for systems reflected with a fissionable material.

CLUTCH THEORY

The theory behind the CLUTCH method for calculating sensitivity coefficients is presented in the SCALE 6.2.2 manual [1]. The portion of this method relevant to the current discussion is that the importance of fission events is determined within an F*(r) function. The importance is determined based on the use of the IFP method during the discarded generations [1]. A significant increase in the number of discarded generations is required to ensure convergence of the F*(r) function compared to convergence of the fission source. Convergence also requires fissions to occur in each voxel of the F* mesh to allow sufficient importance sampling. Ultimately, this led to the discrepant CLUTCH results in reflector sensitivities for systems reflected with fissionable materials. Relatively few fissions occur in the reflector, so a huge number of discarded generations would be required to establish an accurate estimate of its importance. This number was investigated, as discussed in the next section, but satisfactory results were not achieved even after 200 million skipped histories.

PROBLEMATIC BENCHMARKS

As stated previously, CLUTCH calculated inaccurate sensitivities for fissionable isotopes in the reflector for several benchmarks in the VALID library. CLUTCH was only used for fast spectrum systems, though it is expected that thermal systems with fissionable reflectors would experience the same difficulty. These benchmarks included HEU-MET-FAST-030 (HMF-030), HMF-038, HMF-052, HMF-094, IEU-MET-FAST-002 (IMF-002), IMF-007, PU-MET-FAST-006 (PMF-006), and PMF-010. Cases with thin fissionable reflectors did not show large errors, and all cases with non-fissioning reflector materials yielded good sensitivities.

HMF-038 Case 1 was arbitrarily selected as a test case to investigate variations in calculation parameters for this type of system. A 1 cm cubic mesh was used initially since

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the recommended F*(r) mesh size is 1–2 cm [1]. Initially, 500 generations of 10,000 particles were skipped based on the prior experience with CLUTCH calculations [5]. The total sensitivity coefficient for ^{238}U in the depleted uranium reflector was calculated by CLUTCH to be 0.034 ± 1.81%, but DP calculations indicated the actual sensitivity is 0.1107 ± 1.22%. This is an error of almost 70% in the calculated sensitivity.

A series of calculations was performed to investigate the impact of the number of discarded generations used to calculate the F*(r) function on the predicted sensitivity. As mentioned previously, a larger number of discarded generations should improve the results. Calculations were performed with 2,000, 10,000, and 20,000 discarded generations of 10,000 particles each. The number of active generations was varied between 8,000 and 10,000 for each of the calculations in this series. The results provided in Table I show that the error in the ^{238}U is roughly halved between 500 and 2,000 discarded generations. The error is halved again between 2,000 and 10,000 discarded generations to about 15%. The error is only reduced to about 10% by increasing the number of discarded generations to 20,000. While a larger number of discarded generations might eventually yield accurate sensitivities, the study was terminated, as more than 20,000 discarded generations was deemed impractical.

Another series was performed to investigate the effect of the F*(r) mesh size on the calculated sensitivities. Larger mesh should improve the results for the reflector, as more fissions would occur in each voxel. The larger mesh could adversely impact the calculated sensitivity for the fissile portion of the problem if important differences in the local importance are lost with the coarser mesh. This series consisted of 2 cm, 2.5 cm, and 3 cm cubic mesh, with 10,000 discarded generations of 10,000 particles for each mesh. The results are shown in Table I. The error in the ^{238}U sensitivity was reduced from 15% with a 1 cm mesh to approximately 3% with a 2 cm mesh. The error is further reduced to 1.5% for the 2.5 and 3 cm mesh sizes. The change in the sensitivity estimate is statistically equivalent between the 2.5 and 3 cm mesh sizes and is also statistically equivalent to the direct perturbation (reference) sensitivity. The sensitivity estimate for ^{235}U in the central portion of the assembly increased slightly as the mesh size increased, but the difference between the 1 and 3 cm mesh sizes is less than 1.5 standard deviations. The variation is therefore suggestive but may not be statistically significant.

A final calculation was performed with a 3 cm mesh and 1,000 discarded generations. As shown in Table I, the error in the ^{238}U sensitivity in the reflector increased to over 8%. It is clear from this result that, a larger mesh size will not eliminate the problem with the F*(r) function.

TSUNAMI-3D calculations using the IFP method with 3 latent generations generated good sensitivity estimates for ^{235}U, ^{238}U, and ^{9}Be, as shown in Table II. The FOM for these calculations is also on the order of twice the FOM for the CLUTCH calculations for ^{9}Be. This isotope was selected because it has the largest uncertainty in both the IFP and CLUTCH calculations for the three isotopes with large total sensitivities.

TSUNAMI-3D calculations using the MG method were also performed for HMF-038 Case 1. As shown in Table II, the results were also in good agreement with direct perturbation calculations for ^{235}U, ^{238}U, and ^{9}Be. The FOM for the ^{9}Be sensitivity was approximately $^{1}/_{6}$ of the FOM for using IFP and approximately half the of CLUTCH. These results are in agreement with Jones' "Investigation of the Continuous-Energy Sensitivity Methods in SCALE 6.2 Using TSUNAMI-3D" [5], indicating that CE TSUNAMI-3D is more efficient for fast systems than the MG method.

TABLE I. CLUTCH ^{238}U Sensitivities for HMF-038-001

Method	S	Unc. (%)	Error (%)
DP (Reference)	0.1107	1.22	—
1 cm Cubic Mesh, Varying Discarded Generations			
500 discarded	0.0340	1.81	69.3
2,000 discarded	0.0733	0.90	33.8
10,000 discarded	0.0941	0.62	15.1
20,000 discarded	0.0996	0.58	10.1
10,000 Discarded Generations, Varying Mesh Size			
2.0 cm mesh	0.1075	0.54	3.0
2.5 cm mesh	0.1091	0.53	1.5
3.0 cm mesh	0.1091	0.53	1.5
Combined Case			
3.0 cm mesh and 1,000 discarded	0.1014	0.41	8.4

TABLE II. Results for IFP and MG TSUNAMI-3D

Isotope	S	Unc. (%)	Error (%)
CE TSUNAMI-3D IFP			
^{235}U	0.0846	0.6	0.3
^{238}U	0.1099	1.1	0.7
^{9}Be	0.0365	1.8	0.2
MG TSUNAMI-3D			
^{235}U	0.0844	0.7	0.1
^{238}U	0.1089	1.2	1.7
^{9}Be	0.0350	3.5	4.4

GODIVA TO FLATTOP

Following the study on generating accurate sensitivity estimates with thick-reflected systems, a study was conducted to determine the reflector thickness that causes poor results from CLUTCH calculations. The logical endpoints of this study are Godiva (HMF-001)—an unreflected sphere of highly enriched uranium (HEU), and Flattop (HMF-028)—an HEU sphere with an approximately 18 cm thick natural uranium reflector. A series of models was created with reflector thicknesses of 4, 6, 8, 10, 11, and 12 cm to examine sensitivity

calculations as a function of reflector thickness. The critical radius of the HEU sphere was determined for each reflector thickness so the k_{eff} calculated by CE KENO was very close to 1. The radii for Godiva and Flattop were used directly from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook [7] evaluations of the experiments. The critical radii and calculated k_{eff} values are provided in Table III. Sensitivities were calculated using all three TSUNAMI-3D methods and TSUNAMI-1D since it should generate accurate sensitivities for these spherical systems.

TABLE III. Critical Radius and k_{eff} Value for Each Reflector Thickness

Reflector Thickness	**HEU Sphere Radius**	**k_{eff} (ce_v7.1)**	**σ**
0	8.7407	0.99995	0.00007
4	7.040	0.99971	0.00010
6	6.685	1.00008	0.00010
8	6.454	0.99971	0.00010
10	6.309	1.00009	0.00010
11	6.255	1.00008	0.00010
12	6.210	1.00013	0.00010
18.0086	6.1156	1.00312	0.00010

The CLUTCH calculations were performed with 1,000 discarded generations and 2 or 3 latent generations. A 1.5 cm cubic mesh was used for the F*(r) function for Godiva, and a 1 cm cubic mesh was used for the other models. The IFP calculations used 2–5 latent generations. The MG TSUNAMI-3D calculations were run until the uncertainty in the forward k_{eff} was 10 pcm, and the uncertainty in the adjoint k_{eff} was 100 pcm. A 1 cm cubic mesh was used in the MG TSUNAMI-3D calculations. Default parameters were used for the TSUNAMI-1D calculations. Direct perturbation calculations were performed with CE KENO, though MG KENO was also used for Godiva and Flattop. The resulting sensitivity estimates were statistically equivalent for all isotopes tested for both benchmarks.

The two sensitivities of interest in this study are the total sensitivity of ^{235}U in the fissile sphere and ^{238}U in the reflector. The ^{235}U sensitivities are provided in Figure 1 as a function of reflector thickness. It is evident that all four methods generate results that are in good agreement with each other and with the direct perturbation results. The ^{238}U results in Figure 2 show a significant misprediction of the sensitivity using CLUTCH by a thickness of 10 cm. The error increases to almost 10% for Flattop. The other three methods are generally in good agreement with each other and with direct perturbation results. The MG TSUNAMI-3D result for the 12 cm reflector thickness is less than 2 sigma different from the direct perturbation result, the largest difference in the study. A single CLUTCH calculation for Flattop was performed with 10,000 discarded generations and shows good agreement with the other TSUNAMI methods and direct perturbation calculations. Additional runtime for this calculation was approximately 4 hours on 16 cores, an increase by a factor of nearly 4 compared to the 1,000 discarded generation case.

The FOM was determined for ^{235}U in the fissile sphere and ^{238}U in the reflector for each of the three TSUNAMI-3D methods for each reflector thickness. The FOM for ^{235}U is highest for CLUTCH and is generally a factor of 2–10 higher than IFP and a factor of 15–30 higher than MG TSUNAMI-3D. The FOM for ^{238}U is significantly lower than the FOM for ^{235}U for all methods, so it is the more important metric for these calculations. CLUTCH has a higher FOM than IFP or MG TSUNAMI-3D for reflector thicknesses of 8 cm or less. IFP has the highest FOM for 10, 11 and 12 cm thicknesses, and MG TSUNAMI-3D has the highest FOM for Flattop. It appears that the most efficient TSUNAMI-3D method is case dependent, even among very similar fast-spectrum systems.

CONCLUSIONS

Recent experience at Oak Ridge National Laboratory (ORNL) has shown that the CLUTCH method can generate inaccurate sensitivities for thick, fissionable-material reflectors. The two other TSUNAMI-3D methods—IFP and MG—generate accurate results. TSUNAMI-1D also generates accurate results for systems simple enough to be represented accurately. This paper discusses results for a number of benchmark models and some simple spherical models of hypothetical systems. It is expected that the difficulties encountered with these systems would also occur for more complex applications that also have thick fissionable reflectors, such as the GA-4 cask [8]. Users should exercise caution when executing TSUNAMI sequences and confirm results using direct perturbation calculations.

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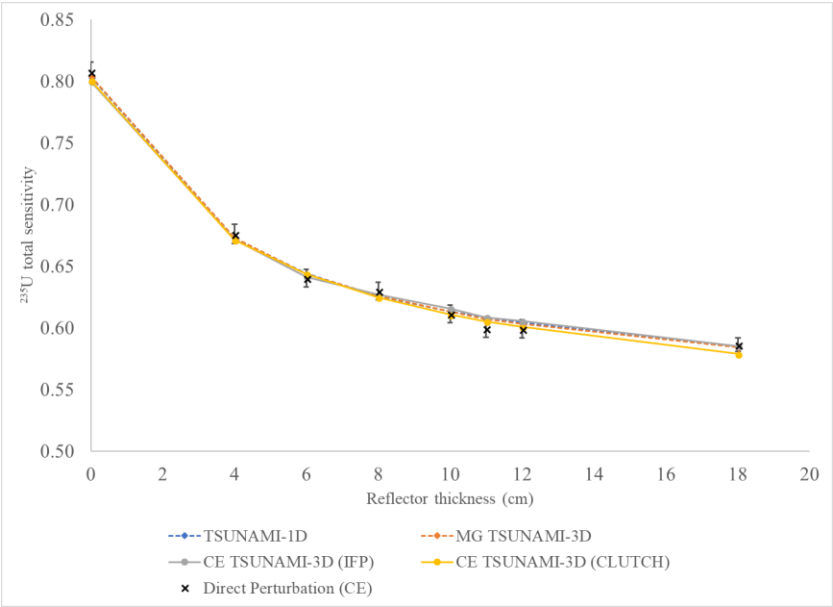

Fig. 1. Fissile sphere ^{235}U total sensitivity as a function of reflector thickness.

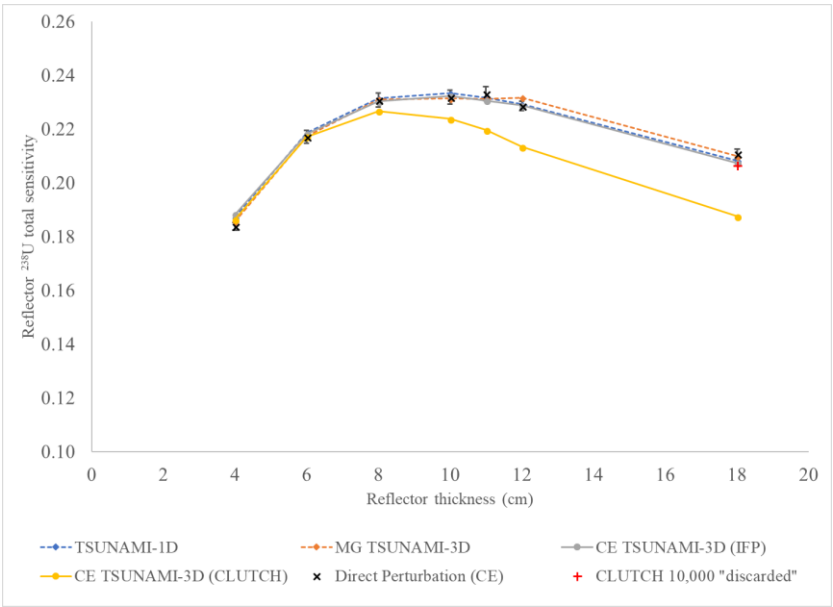

Fig. 2. Reflector ^{238}U total sensitivity as a function of reflector thickness.