A Case Study in the Application of TSUNAMI-3D – Part 3, Continuous Energy – Iterative Fission Probability Method

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INTRODUCTION

The use of the sensitivity and uncertainty tool suite within SCALE, which is known as the TSUNAMI suite, has grown following its initial introduction more than a decade ago. Proper use of this tool provides a more complete understanding of system responses to small perturbations such as those related to nuclear cross section uncertainties. The sensitivities can also be used to quantify the similarity of two systems based on their eigenvalue responses. For example, calculated sensitivities can be combined with cross section uncertainties to determine the similarity index c_k [1,2]. c_k should be viewed as fractional amount of shared nuclear data uncertainty. The generation of sensitivity data is encouraged in the review process for new critical experiment requests sponsored by the US Department of Energy (DOE) Nuclear Criticality Safety Program (NCSP) to demonstrate that the proposed experiment will satisfy the identified data need [3]. Many analysts use this process, but many have not received proper training in the use of the TSUNAMI tools.

The first step in using TSUNAMI tools is to generate a sensitivity data file (SDF) containing all the energy-dependent sensitivity data that has been generated for a model. The SDF is typically generated from a three-dimensional (3D) model using either KENO V.a or KENO-VI code within the TSUNAMI-3D sequence. The sensitivity data generated in TSUNAMI-3D must be accurate for correct quantification of system similarity or for any other use. The sensitivities calculated by TSUNAMI can be affected by many of the input parameters, cross section processing models, and geometry modeling techniques used within the TSUNAMI-3D input. Fortunately, the total sensitivity of the most important nuclides can be confirmed simply by using direct perturbation (DP) calculations. Confirming the total sensitivity of these important nuclides provides confidence that the flux and importance function calculated within the TSUNAMI sequence will yield accurate sensitivities for all nuclides, reactions, and energies of interest. This process is essentially identical for multigroup (MG) and continuous-energy (CE) methods introduced in SCALE 6.2 [2].

This paper discusses the use of DP calculations and provides a case study in their use to confirm accurate sensitivities generated by CE-TSUNAMI using the iterative fission probability (IFP) method [2] for a specific benchmark experiment. Companion papers present similar case studies applying the MG-TSUNAMI [4] and CE-TSUNAMI contribution linked sensitivity/uncertainty estimation via track length importance characterization (CLUTCH) [5] methodologies to the same critical experiment.

DP CALCULATIONS

DP calculations are used to confirm the total sensitivity coefficient for nuclides of interest within specific mixtures and or throughout the entire used in the model. The total sensitivity is confirmed because a change introduced to the material number density changes the macroscopic cross section in a manner equivalent to assessing the system's sensitivity to changes in the microscopic cross section. TSUNAMI-3D uses perturbation theory to calculate the sensitivity and does not actually perturb cross sections in the model. The DP calculations are performed in the same transport code that is used in the TSUNAMI model. These transport codes are XSDRN-PM for TSUNAMI-1D, NEWT for TSUNAMI-2D, and KENO V.a or KENO-VI for TSUNAMI-3D. In this case study, KENO V.a is used in TSUNAMI-3D and in the associated DP calculations.

An important facet of DP calculations is the selection of nuclides, elements, and/or materials of interest. Generally, this should include at least the primary fissionable and moderating species. Additionally, materials or nuclides of special interest—such as the primary absorber for a poison relied on for safety—can be used if their sensitivity is high enough. It is also advantageous to select materials from a range of geometric regions to ensure solution convergence in all portions of a model. Selection of high-sensitivity candidates simplifies the DP calculations by reducing the relative uncertainty in the sensitivity due to the Monte Carlo uncertainty.

The magnitude of the density change used in the DP must also be selected. Experience has shown that a perturbation that is selected to cause a change of ±0.5% Δk provides a good balance between a large enough perturbation to yield accurate results while still being a small enough difference to generate a linear response. Base line estimates of the density change needed to include a 0.5% Δk are made using the TSUNAMI calculated sensitivity. The nominal k_{eff} value from a KENO model is used along with these two perturbed results to determine the sensitivity as the slope of a fit to the k_{eff} versus the density plot. Additional points can be used to reduce the uncertainty of the DP sensitivity or to investigate potential

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nonlinear behavior. Figure 1 shows an example plot of the weighted linear least squares fit of three points used to determine the DP sensitivity for an example case. The slope of the trend line is the sensitivity, and the uncertainty of this fit can also be calculated to provide the uncertainty in the DP sensitivity. Both of these quantities should be evaluated at the nominal density, which is shown in Fig. 1 as a Δρ of 0. Sensitivities of 0.02 and higher lead to density perturbations of 25% or less, which generally remain in the linear range.

It is desirable for the differences between TSUNAMI and DP sensitivities to be less than 5%, less than 0.01 in absolute sensitivity, and/or less than 2 standard deviations using the combined uncertainties. A sensitivity profile is generally considered acceptable for use when it meets two of these three criteria. DP uncertainties of 1–2% are highly desirable for highly reliable confirmation of sensitivities; this eliminates an unnecessary source of noise in the calculations. For cases in which DP calculations and TSUNAMI-generated sensitivities disagree by margins greater than those in the established guidelines, it is advisable to first check the DP calculations due to the relative ease of rerunning them and the relatively high error rate associated with manipulation of text files. If the DP calculations are correct, then the TSUNAMI calculations must be examined. Generally, CE TSUNAMI-IFP discrepancies can be resolved by increasing the number of latent generations or increasing the total number of active histories.

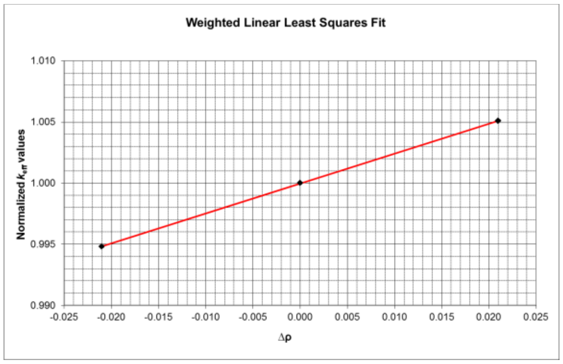

Fig. 1. Example DP result.

EXPERIMENT DESCRIPTION

The benchmark experiment selected in this case study—HEU-MET-MIXED-017 (HMM-017) [6]—was selected because of prior difficulty in generating accurate sensitivities in similar systems. The experiment was performed in 2009 at the Russian Federation Nuclear Center's Institute of Technical Physics (VNIITF) using a vertical lift machine. The experiment contains a cylindrical core made up of disks of highly enriched uranium (HEU), polyethylene, and tungsten. The cylindrical core has polyethylene top and bottom reflectors and is surrounded by an annular reflector of polyethylene. A schematic of the experiment is provided in Fig. 2.

Configurations such as the one presented here are very challenging for MG calculations because of the high degree of both axial and radial heterogeneity. The cross section processing models available within SCALE are incapable of modeling this level of heterogeneity. Explicit representation of the axial layering is possible in a 1D model, but the effect of the radial reflector cannot be captured. The cross section processing difficulties encountered in modeling configurations such as these make CE methods particularly attractive. The axial layering and radial reflector present in HMM-017 bear some resemblance to some of the TEX experiments currently being designed at Lawrence Livermore National Laboratory [7], indicating that the difficulties encountered with this system will likely apply to that system, as well. In TSUNAMI-3D models, the cross section processing calculations also determine the implicit portion of the sensitivity coefficients. This is the portion that represents the effect of cross sections on each other during the self-shielding process.

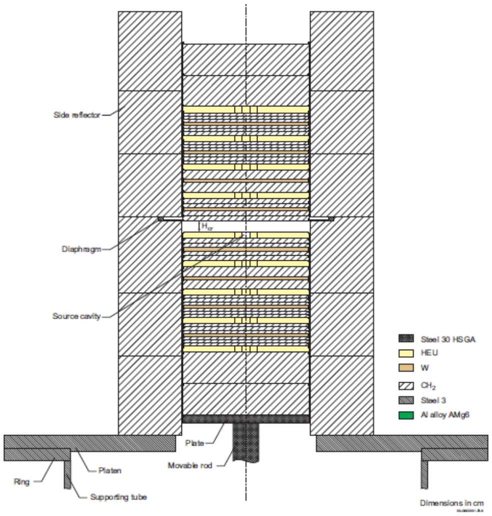

Fig. 2. Schematic representation of HMM-017 [7].

RESULTS

To demonstrate the process, an initial CE TSUNAMI-IFP calculation was performed with 3,000 active generations (200 skipped) of 10,000 particle histories per generation using 10 latent generations for the importance calculation. The comparison of CE TSUNAMI-3D-IFP and DP sensitivities for this model is shown in Table I. These results showed acceptable agreement with the previously mentioned criteria; therefore, the CE TSUNAMI agreement with the DPs is acceptable for each nuclide.

Table I. Sensitivity Comparisons for Base Model

Element or Nuclide	ΔS (%)	ΔS (σ)	ΔS (abs)
C (refl)	1.45	0.93	-0.0005
C (disk)	0.25	0.08	-0.0001
H (disk)	1.70	0.48	0.0010
^{235}U (disk)	0.42	0.82	-0.0012
^{182}W	3.93	1.84	0.0006
^{186}W	2.82	1.73	0.0006

Even though these results are within the desired ranges, it is preferred to obtain an axial profile of the sensitivities for this model to further investigate the efficacy of the IFP method. Therefore, the individual sensitivities for each disk were compared to DP calculations for each identical disk of HEU, allowing for a more detailed comparisons. The comparison of TSUNAMI and DP sensitivities for each disk is shown in Table II. Even though the largest difference in standard deviations is greater than two standard deviations for ^{235}U in disk 9 (top disk), the CE TSUNAMI sensitivity results are still considered consistent with the DPs due to the consistency of the other metrics.

Table II. Detailed Sensitivity Comparisons

Isotope	ΔS (%)	ΔS (σ)	ΔS (abs)
^{235}U (disk 1)	2.26	1.16	-0.0003
^{235}U (disk 2)	0.77	0.49	-0.0002
^{235}U (disk 3)	0.19	0.13	0.0001
^{235}U (disk 4)	1.38	1.02	0.0006
^{235}U (disk 5)	1.40	1.03	-0.0006
^{235}U (disk 6)	0.69	0.50	0.0003
^{235}U (disk 7)	0.10	0.07	0.0000
^{235}U (disk 8)	2.51	1.57	-0.0006
^{235}U (disk 9)	3.97	2.03	-0.0005

Calculations were also performed with the same number of active neutron histories but with 5 and 20 latent generations. The increase and decrease in the number of latent generations resulted in small, random changes in the calculated sensitivity coefficients. It was observed that the uncertainties on the sensitivity coefficients are 25% smaller for the 5 latent generation case and 37% larger for the 20 latent generation case when compared to the 10 latent generation case. It is thought that the larger number of latent generations decreases the total number of neutron histories that contribute to the importance calculation, while improving the quality of the information obtained from each contributing history, thus leading to higher uncertainties in what are likely more accurate answers. The impact of the number of latent generations on the calculation is an area in need of further investigation, is likely system dependent, and is beyond the scope of this paper.

An additional check was performed in this case by plotting the ^{235}U sensitivity for each disk. These results are shown in Fig. 3 and indicate a largely cosine-shaped distribution. This is expected based on the nearly symmetric distribution of HEU, tungsten, and polyethylene disks and reflectors in the assembly.

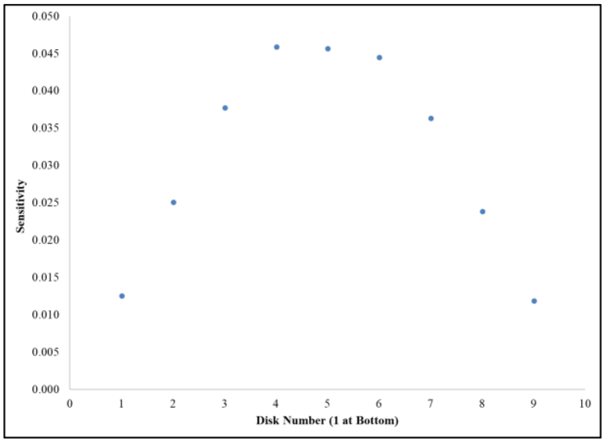

Fig. 3. Axial profile of ^{235}U sensitivity by disk

Figure 4 presents comparisons of the MG, CE TSUNAMI-CLUTCH, CE TSUNAMI-IFP and DP results for nuclide sensitivities having an absolute magnitude of ~0.02 or greater. The x-axis in Fig. 4 represents the ^{235}U fuel disks, starting from #1 at the bottom of the configuration to #9 at the top. As expected, the shape of the sensitivities matches well with the probable distribution of fission neutrons as a function of position. The MG and CE TSUNAMI-3D and DP results presented in Fig. 4 are considered acceptably consistent.

CONCLUSIONS

The purpose of this paper is to demonstrate the proper use of DP calculations to confirm sensitivities calculated using the CE TSUNAMI suite within SCALE. A case study has been presented for the HMM-017 experiment in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook [6] with CE TSUNAMI calculations. Previously published papers [4] and [5] present the same experiment with sensitivities calculated with MG TSUNAMI and CE TSUNAMI-CLUTCH. Overall, the sensitivity results reported by all versions of TSUNAMI are consistent for the HMM-017-001 model. A flowchart illustrating the TSUNAMI and DP process is provided in Fig. 5. The use of DP calculations to confirm TSUNAMI sensitivities is an essential step in the process of SDF generation.

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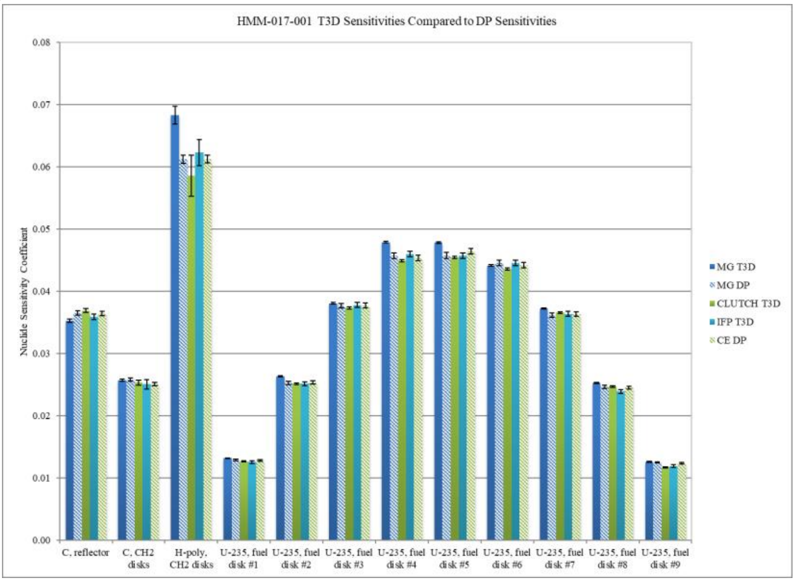

Fig. 4. TSUNAMI-3D and DP sensitivity comparisons for representative HMM-017-001 nuclides.

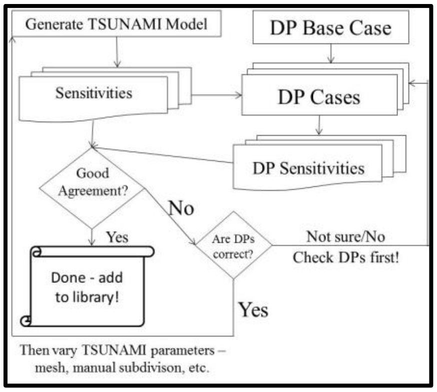

Fig. 5. Process for TSUNAMI calculations with DP checks.