Performing k_{eff} Validation of As-Loaded Criticality Safety Calculations Using UNF-ST&DARDS: Sensitivity Calculations *

W. J. Marshall, J. B. Clarity, and K. Banerjee

Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6170, USA, marshallwj@ornl.gov

INTRODUCTION

The general method for performing validation of as-loaded criticality safety calculations using UNF-ST&DARDS is presented in a paper by Clarity [1], which includes a description of the UNF-ST&DARDS system. Proof-of-principle analyses were performed in the summer of 2019 for MPC-32 dual purpose canisters (DPCs) containing pressurized water reactor (PWR) fuel assemblies. Summaries of these results are presented in this and a companion paper for this conference [2]. The current paper describes the TSUNAMI-3D [3] calculations performed to generate sensitivity data, and the companion paper discusses the selection of critical experiments applicable for validation of the 11 MPC-32 DPCs considered.

The generation of sensitivity data for as-loaded spent nuclear fuel (SNF) DPCs is a challenge given the detailed model of the fuel compositions generated by UNF-ST&DARDS. Each fuel assembly is modeled with its own irradiation history in 18 axial nodes, unless the fuel assembly is damaged and thus considered as fresh by design basis. This results in a set of 576 fuel compositions, each of which must be processed separately in a multigroup (MG) calculation. Therefore, a continuous-energy (CE) TSUNAMI-3D method was chosen to alleviate this challenge. Two CE TSUNAMI-3D methods are available in SCALE 6.2.3: the iterated fission probability (IFP) and contributon-linked eigenvalue sensitivity/uncertainty estimation via track-length importance characterization (CLUTCH). Since the IFP method is not feasible because of memory requirements associated with its implementation in SCALE, the CLUTCH method was selected for these calculations. CLUTCH has been implemented in SCALE in parallel, allowing long calculations to be performed in reasonable timeframes.

The two primary user inputs necessary for CLUTCH calculations are the F*(r) mesh and the number of latent generations used in determining the F*(r) function. This F*(r) function is used as the importance function for fission chains originating in a given volume element (voxel), and it is calculated using the IFP method in the skipped generations. A large number of skipped generations is thus required to ensure accurate calculation of this importance function. In these calculations, 500 generations were used to calculate the F*(r) function. For more information regarding the calculation of F*(r), see Jones [4]. The remainder of this paper is focused on the selection of the F*(r) mesh and the number of latent generations.

F*(r) MESH SELECTION

As implemented in SCALE 6.2.3, the CLUTCH method requires a 3D cartesian mesh within which the importance of fission chains is tallied based on the voxel in which the initial fission occurs. The entire neutron history is assigned a weight based on the location of the fission that gave birth to the neutron. This method also allows for calculation of sensitivities for nonfission reactions. As mentioned previously, the description of this mesh is one of the primary parameters that a user must determine to generate accurate sensitivity coefficients.

Generic guidance for determining the F*(r) mesh is to use a uniform cubic mesh of 1–3 cm on a side [5]. This guidance was developed using critical experiments, which tend to be significantly smaller systems than SNF DPCs. Several histories must traverse each voxel to provide enough tallies for sufficiently low uncertainties in the F*(r) function. This presents a significant burden for systems as large as a DPC. A review of the F*(r) function revealed that (1) the central assemblies in the MPC-32 DPC dominate the importance function, and (2) the importance is nearly uniform radially in these central storage locations.

Based on this information, the radial mesh for F*(r) was coarsened to ¼ of the storage cell's size. The mesh spacing in the x and y directions is half the storage cell size; therefore, each storage cell is divided into 4 mesh intervals radially. Figure 1 is a radial plot of the F*(r) function for the highest importance axial level in a specific DPC model showing the mesh. The importance in each cell is largely uniform and is primarily driven by the fuel assembly stored in that location. The adjacent storage locations are a secondary influence on the importance of central storage locations. The importance of storage locations along the periphery of the DPC are more strongly impacted by neutron leakage.

Axially, a variable mesh was developed with larger mesh spacing in lower elevation, low importance regions of the DPC. The fuel is located within the model at axial positions extending from z=22.5425 to z=388.3025. The top two feet of the fuel is divided into ten 2.4-inch axial mesh intervals to capture the gradient of the importance function near the top end of the fuel. The highest of these intervals was divided by an additional plane (at

* Notice: This manuscript has been authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the US Department of Energy (DOE). The US government retains and the publisher, by accepting the article for publication, acknowledges that the US government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this manuscript, or allow others to do so, for US government purposes. DOE will provide public access to these results of federally sponsored research in accordance with the DOE Public Access Plan (http://energy.gov/downloads/doe-public-access-plan).

z=386.7025 cm) that was inadvertently not removed during mesh refinement studies. The axial mesh locations are listed in Table I.

The confirmation of the accuracy of the TSUNAMI-3D calculated sensitivities by direct perturbation (DP) calculations confirms that the F*(r) mesh is sufficiently refined. The results for these comparisons are not presented here due to space limitations. The calculated total ^{235}U sensitivity is within 3% of the DP results in all cases. All total ^{238}U sensitivities are within 4%, and total ^{10}B sensitivities are within 5.5%. Total ^{1}H sensitivities are all within 8%, however better agreement in outlier cases is desired. The ^{1}H results for 8 of the 11 DPCs considered agree with DP results, with less than 5% difference. Overall, these sensitivities are judged to be sufficiently close to the DP results for use in critical experiment selection [6].

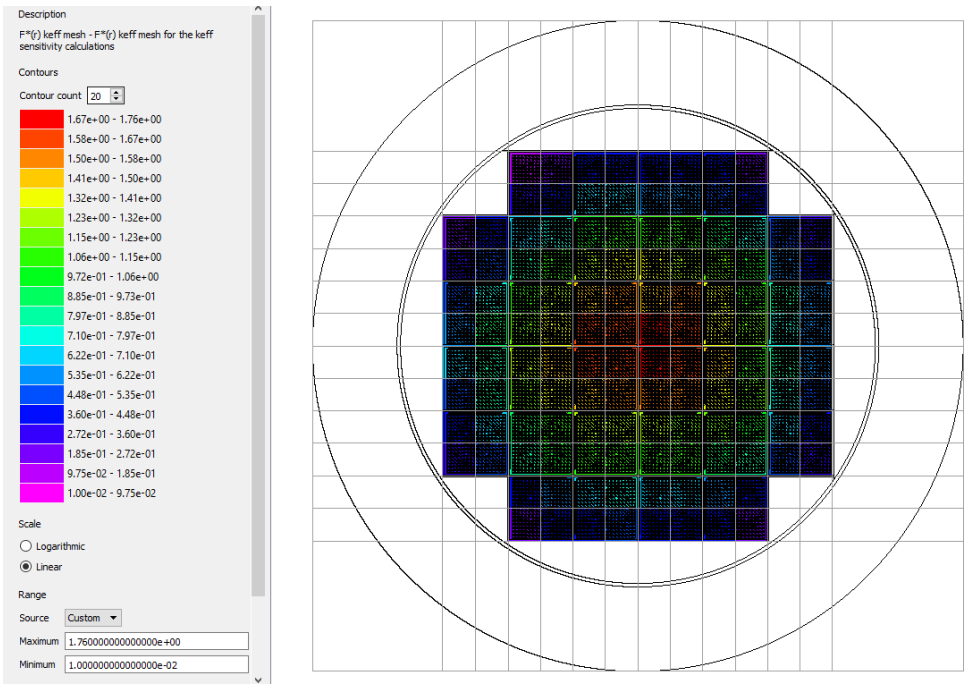

Fig. 1. Cross sectional plot of F*(r) mesh and function.

TABLE I. Axial (z) Planes for F*(r) Mesh (cm)

-61.0005	0.0000	22.5425	144.4625	266.3825	307.0225	327.3425
333.4385	339.5345	345.6305	351.7265	357.8225	363.9185	370.0145
376.1105	382.2065	386.7025	388.3025	410.8450	448.3100	480.3105

NUMBER OF LATENT GENERATIONS

The other important parameter for CLUTCH calculations is the number of latent generations used to determine the F*(r) function. The CLUTCH method uses the IFP method to determine the value of the F*(r) function in each voxel. The IFP method determines importance by tracking the number of neutrons in the system that are descended from each fission chain. This assessment of the progeny is performed some number of generations after the fission that begins the chain: this number is known as the *number of latent generations*. Higher numbers of latent generations should yield more accurate results, but they could result in fewer fission chains tallying any importance at all. Having fewer chains that last long enough to contribute to the importance tally leads to the need for larger numbers of histories to achieve the desired uncertainty in the importance function. Thus, a balance between long run-times and greater confidence in the accuracy of the calculation is required. DP calculations can be used to generate confidence in the tallied results. However, these calculations are performed on the final CLUTCH-calculated sensitivities instead of the F*(r) values. Guidance on the number of latent generations is provided in the SCALE manual. The default value is 10 latent generations, and 20 latent generations is described as "typically a conservative number" [3]. The number of latent generations is independent of the total number of skipped generations used to calculate the F*(r) function; enough generations needs to be included in this portion of

the calculation to generate a sufficiently converged estimate of the importance function. All calculations discussed here skipped 500 generations of 50,000 neutron histories.

Initial calculations using 5 and 10 latent generations did not yield good agreement between TSUNAMI-3D sensitivities and the reference DP results, especially for ^{1}H. After other sensitivity studies did not improve agreement, the number of latent generations was increased. Agreement with DP results improved, as shown in Figure 2 for total ^{1}H and in Figure 3 for ^{235}U, summed over the 4 mixtures with the highest total ^{235}U sensitivity. In each figure, the best estimate TSUNAMI-3D result is shown with blue dots, and the one-sigma uncertainty bars are shown in black. The reference DP result is shown as a green line, since the TSUNAMI-3D parameters have no impact on the reference result. Figure 2 shows the TSUNAMI-3D sensitivity approaching the reference result as the number of latent generations is increased. The estimate changes significantly between 5 and 20 latent generations and continues to increase at 30. Very slight increases may be seen between 30 and 60 latent generations. Whereas these changes are not individually statistically significant, they do form a steady trend. The trend is more remarkable for ^{235}U, as shown in Figure 3. These sensitivities have much smaller uncertainties, so changes in the sensitivities are more likely to be statistically significant. These results indicate that there is some change between 30 and 40 latent generations, but none above 40.

These results are interesting due to the number of latent generations that appear to be necessary to yield an asymptotic estimate of the sensitivity. As mentioned previously, most of the guidance provided for using CE TSUNAMI-3D methods is based on models of critical experiments, which are much smaller systems than DPCs. It is not clear whether these results indicate the complexity of the system or its physical size. It is also unclear if an IFP calculation would require such a large number of latent generations. The SCALE implementation of IFP requires too much memory to allow for such a large number of latent generations. Future calculations using Shift could be used to investigate whether a larger number of latent generations is also needed for IFP.

It should be noted that 30 latent generations were used to generate sensitivities used for these models. The results were judged to be sufficiently accurate for the purposes of critical experiment selection, as discussed previously. The calculations with 40, 50, and 60 latent generations were performed later to further investigate the trends as reported in this paper.

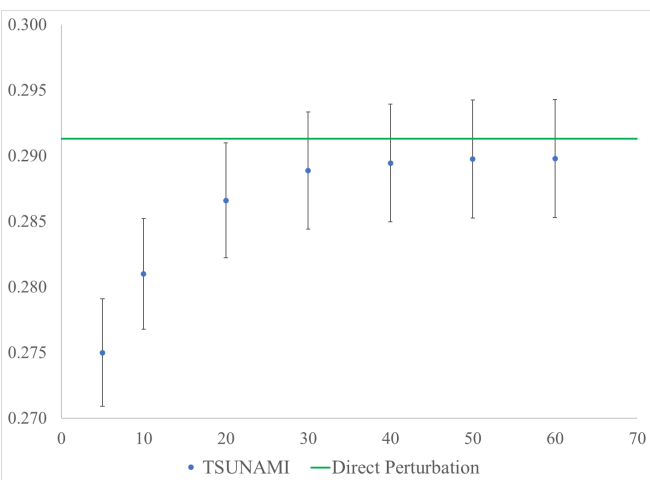

Fig. 2. Total ^{1}H sensitivity as a function of the number of latent generations.

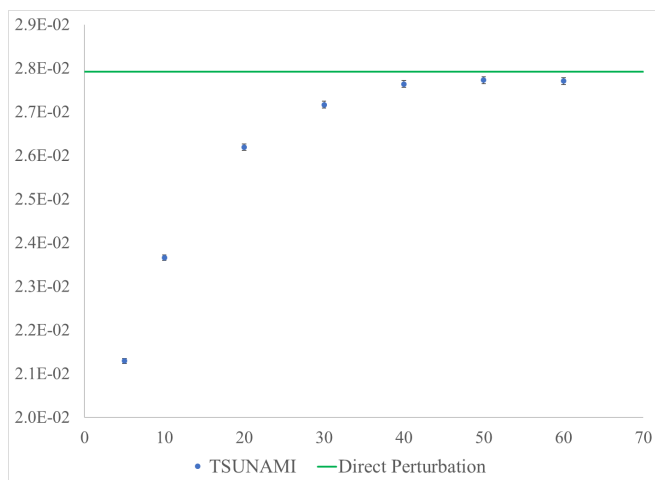

Fig. 3. Total ^{235}U sensitivity summed over the four highest sensitivity mixtures as a function of the number of latent generations.

CONCLUSION

Sensitivity calculations were performed in support of validation of as-loaded criticality safety calculations in UNF-ST&DARDS. These calculations represent some of the largest, and most complex sensitivity calculations performed to date in terms of system size, and especially in terms of the number of different mixtures included in the model. The size and complexity of these models essentially precluded the use of MG TSUNAMI-3D and the CE TSUNAMI-3D IFP method in its current implementation. The CLUTCH method was used to calculate sensitivities for these models using CE TSUNAMI-3D.

Two aspects of the CLUTCH calculations are reviewed in this paper: the F*(r) mesh, and the number of latent generations. An acceptable F*(r) mesh was determined to have a quarter storage cell radial mesh and a coarse axial mesh. Additional meshes were added in the high-importance regions of the top end of the fuel assemblies, as shown in Table I. This mesh deviates

significantly from generic guidance for use of the CLUTCH method. The number of latent generations required for accurate sensitivity calculations are also reviewed herein. The results used for critical experiment selection, presented in a companion paper [2], used 30 latent generations. Results presented here indicate that slightly better agreement can be achieved with 40 latent generations, and there are no apparent indications that increases beyond 40 will yield improved results. As with the F*(r) mesh, the use of 30 latent generations deviates somewhat from published recommendations on the number of latent generations necessary for accurate calculations. It is not clear if this large number of latent generations also applies to the IFP method.

FUTURE WORK

Future work could be productive in a number of areas. Examining the number of latent generations needed for accurate results using the IFP method could be investigated in future SCALE releases using the Shift Monte Carlo code. The relationships between accurate sensitivity calculations and the F*(r) mesh and the uncertainties of the F*(r) function are still not well understood. At this point, it seems unlikely that additional study will reveal generic guidance, but these relationships will likely need to be established on a case-by-case basis or perhaps for classes of similar models.

Future work in this area for UNF-ST&DARDS will focus on integration of these TSUNAMI-3D parameters for automatic calculations and validation. More information on experiment selection is included in Rearden and Jessee's *SCALE Code System* [2]. The general approaches identified here for accurate sensitivity calculations for MPC-32 DPCs must be tested for use with additional DPC designs. Expansion to BWR SNF will also be an important area of future work.

ACKNOWLEDGMENT

Development of UNF-ST&DARDS criticality analysis capability was accomplished with funding provided by the US Department of Energy (DOE) Office of Nuclear Energy (NE). The preparation and presentation of this paper was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.

REFERENCES

1. J. CLARITY, W. MARSHALL, K. BANERJEE, and J. SCAGLIONE, "A Method for Performing k_{eff} Validation of As-Loaded Criticality Safety Calculations Using UNF-ST&DARDS," *Trans. Am. Nucl. Soc.* **120**, 504–507 (2019).
2. W. MARSHALL, J. CLARITY, and K. BANERJEE, "Performing k_{eff} Validation of As-Loaded Criticality Safety Calculations using UNF-ST&DARDS: Applicable Experiment Selection," *Trans. Am. Nucl. Soc.* **122**, (anticipated in 2020).
3. B. REARDEN and M. JESSEE, Editors, *SCALE Code System*, ORNL/TM-2005/39, Version 6.2.3, Oak Ridge National Laboratory (2017).
4. E. JONES, "User Perspective and Analysis of the Continuous-Energy Sensitivity Methods in SCALE 6.2 Using TSUNAMI-3D," Master's Thesis, University of Tennessee, Knoxville, Tennessee (2015).
5. C. PERFETTI and B. REARDEN, "Development of a SCALE Tool for Continuous-Energy Eigenvalue Sensitivity Coefficient Calculations," Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013 (SNA + MC 2013), La Cité des Sciences et de l'Industrie, Paris, France (2013).
6. W. MARSHALL, E. JONES, B. REARDEN, and M. DUNN, "A Case Study in the Application of TSUNAMI-3D – Part 1, Multigroup," *Trans. Am. Nucl. Soc.* **115**, 673–676 (2016).