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SENSITIVITY COEFFICIENT GENERATION FOR A BURNUP CREDIT CASK MODEL USING TSUNAMI-3D

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ABSTRACT

The evolution of a complex criticality model for a burnup credit shipping cask to an accurate TSUNAMI-3D model for eigenvalue sensitivity coefficient generation is detailed in this paper. TSUNAMI-3D is a Monte Carlo–based eigenvalue sensitivity analysis sequence that was released with SCALE 5. In the criticality model, 32 fuel assemblies, each with 18 axial zones with differing depletion-dependent compositions, are placed in a generic burnup credit cask, referred to as the GBC-32, in a fully flooded condition. The selection of various combinations of options for TSUNAMI-3D and their effect on computational requirements and the validity of the sensitivity coefficients, relative to direct difference calculation results, are described. Accurate modeling of this system required the use of prototypic codes developed for the next release of SCALE.

Key Words: TSUNAMI, STARBUCS, KENO, Sensitivity, Burnup Credit

1 INTRODUCTION

Historically, criticality safety analyses for commercial light-water-reactor spent nuclear fuel (SNF) storage and transportation casks have assumed the SNF to be fresh (unirradiated) with uniform isotopic compositions corresponding to the maximum allowable enrichment. This *fresh-fuel assumption* provides a simple bounding approach to the criticality analysis and eliminates concerns related to the fuel operating history. However, because this assumption ignores the decrease in reactivity as a result of irradiation, it is very conservative and can result in a significant reduction in SNF capacity for a given cask volume. Numerous publications, an extensive set of which is listed in the reference section of NUREG/CR-6800 [1], have demonstrated that increases in SNF cask capacities from the use of burnup credit can enable a reduction in the number of casks and shipments and thus have notable financial benefits while providing a risk-based approach to improving safety. The concept of taking credit for the reduction in reactivity due to irradiation of nuclear fuel (i.e., fuel burnup) is commonly referred to as *burnup credit*. The reduction in reactivity that occurs with fuel burnup is due to the change in concentration (net reduction) of fissile nuclides and the production of parasitic neutron-absorbing nuclides (nonfissile actinides and fission products).

TSUNAMI-3D [2] is a Monte Carlo–based eigenvalue sensitivity analysis sequence that was released with SCALE 5. This software tool permits energy-, mixture-, nuclide- and region-dependent examination of the sensitivity of the system k_{eff} to variations in macroscopic cross sections of modeled materials. TSUNAMI-3D uses first-order linear-perturbation theory to

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produce sensitivity coefficients. As such, the sensitivity coefficients are valid only for small perturbations. The sensitivity profiles generated for a particular system of interest may be compared with the sensitivity profiles for critical experiments used to generate subcritical limits in validation studies. Such comparisons enable the analyst to reach conclusions regarding the adequacy of the set of critical experiments used in the validation study. The analyst's selection of modeling strategies and TSUNAMI-3D input parameters can significantly affect the sensitivity profiles generated by TSUNAMI-3D for both the application-specific model and the criticality experiment models used in the supporting validation study. Thus, the importance of performing a thorough set of direct perturbation (DP) calculations to verify the accuracy of the TSUNAMI-3D sensitivity data cannot be overemphasized. As is discussed below, care must also be exercised in performing these DP calculations.

Work is being performed at Oak Ridge National Laboratory to generate recommendations and develop computational methods related to taking credit for the in-reactor burnup of commercial nuclear fuel during out-of-reactor storage and transport. Numerous studies are available in the open literature demonstrating the benefits of burnup credit and reviewing associated technical issues. The purpose of this paper is to share experiences associated with the use of two relevant computational tools, STARBUCS and TSUNAMI-3D, which became publicly available with the release of SCALE version 5.0. Subsequent sections of this paper describe development of the burnup credit cask model, calculation of sensitivity coefficients using DP methods, calculation of sensitivity coefficients and energy-dependent profiles using TSUNAMI-3D, comparison of some sensitivity coefficients and energy-dependent profiles generated for a few critical experiments and for the SNF in the flooded-cask geometry, and planned code developments for the SCALE system.

2 BURNUP CREDIT CASK MODEL AND METHODS

A generic cask model with a 32 pressurized-water-reactor (PWR) assembly capacity was developed by Wagner and is described in NUREG/CR-6747 [3]. This model, referred to as the GBC-32, was created to serve as a computational benchmark. The features of GBC-32 include 32 cells with 365.76-cm-tall and 19.05-cm-wide Boral (0.0225 g $^{10}B/cm^2$) panels between and on the external faces of each cell. The cell walls are constructed of stainless steel having inner dimensions of 22 × 22 cm and are spaced on 23.76-cm centers. The cells sit 15 cm above the bottom of a stainless steel cask having an inner radius of 87.5 cm and internal height of 410.76 cm. The radial thickness of the side walls is 20 cm, and the cask bottom and lid are 30 cm thick.

For purposes of the analyses documented in this paper, the cask was modeled as loaded with Westinghouse 17 × 17 Optimized Fuel Assemblies (W17×17OFA). The dimensions for the W17×17OFA were taken from Table 3 of reference 3. The interior of the cask was modeled as if it were filled with water.

The fuel had an initial enrichment of 4 wt % ^{235}U and was burned to 40 GWd/MTU. The STARBUCS sequence in SCALE 5 was used to generate 18 axial location-dependent burned fuel compositions. The STARBUCS sequence and available input parameters are discussed in reference 4. The normalized burnup profile from Table 5 of reference 3 was used. The fuel burnup was modeled at a power density of 40 MW/MTU for 1000 days, with a post-shutdown cooling period of 5 years. From the depletion calculations, fuel compositions for the following nuclides were retained for the criticality calculations: ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{243}Am, ^{95}Mo, ^{99}Tc, ^{101}Ru, ^{103}Rh, ^{109}Ag, ^{133}Cs, ^{147}Sm, ^{149}Sm, ^{150}Sm, ^{151}Sm, ^{152}Sm, ^{143}Nd, ^{145}Nd, ^{151}Eu, ^{153}Eu, and ^{155}Gd. The fuel burnup calculations model the depletion of the ^{235}U and the in-growth of plutonium and fission product nuclides.

Under normal conditions, fuel burned in a PWR accumulates an axial burnup profile that may be characterized as a chopped cosine shape that is slightly skewed toward the bottom. Thus, the ^{235}U is depleted, and the actinides and fission products are created more in the lower-middle axial region than on the ends of the fuel. This axial burnup shape is caused, in part, by axial neutron leakage and the increase in moderator and fuel temperatures as the moderator moves from the bottom to the top inside the reactor core when it is producing power. In storage or transport geometries, no such temperature gradient exists. Consequently, the axial fission distribution of stored spent PWR fuel is very highly skewed to the top of the fuel assembly. Calculations of the burned fuel in the GBC-32 cask show that the top 81 cm (32 in.) of the fuel has 95% of the fission density and the top 41 cm (16 in.) has 70% of the fission density. This information is important in performing the TSUNAMI-3D calculations.

The STARBUCS sequence uses the ORIGEN-ARP sequence to calculate the burned fuel compositions and then creates an input deck and runs a criticality calculation. STARBUCS can perform criticality calculations using KENO V.a or KENO VI. Currently, TSUNAMI-3D works only with KENO V.a.

During the STARBUCS sequence, a criticality sequence input file, called ***sysin2***, is created in the user's temporary working directory. This input file, which includes the depleted fuel compositions, is needed for both TSUNAMI-3D and DP calculations. When the SCALE ***batch5*** command is used, SCALE normally deletes the temporary directory after the calculation is completed. The ***sysin2*** file may be saved using one of several methods. The input file may be extracted from the STARBUCS output file. After STARBUCS finishes the depletion calculations and starts the criticality calculations, the user may locate the appropriate temporary directory and copy ***sysin2*** to a location outside the temporary directory. The user may also include an "-r" flag in the ***batch5*** command line, which tells SCALE not to delete the temporary working area. The user may then copy ***sysin2*** from the temporary directory after the job is finished. The last method is to include "shell" commands at the end of the STARBUCS input deck to copy ***sysin2*** back to the user's working directory. On a UNIX workstation, the shell commands are the following:

```
#shell
cp  sysin2  ${root}.buc.input
end
```

This command will copy the ***sysin2*** file back to the same location as the input and output files and appends the extension ***.buc.input*** to the same base name assigned to the original input file. On a Windows XP computer, the shell commands are the following:

```
#shell
copy  sysin2  "%RTNDIR%\%TMPVAR%.buc.input"
end
```

As discussed in Section 4, memory and hard drive space requirements may limit the size and complexity of models that may be evaluated using TSUNAMI-3D.

As is noted in the SCALE documentation, the TSUNAMI-3D version distributed with SCALE 5.0 will not work if the model has more than 50 nuclides that have resonance information. Each occurrence of the same resonance nuclide in multiple mixtures is counted toward this limit. The GBC-32 cask model included different mixtures of uranium, plutonium, other actinides, and 15 fission products in each of 18 axial zones. There were in excess of 500 resonance nuclides in all mixtures. Consequently, special development versions of some of the TSUNAMI-3D sequence programs were created by the SCALE development staff to support this work. The 50-resonance-nuclide limitation will be removed in SCALE 5.1. However, users will need to keep this 50-nuclide limit in mind during model development with SCALE 5.0.

3 DIRECT PERTURBATION CALCULATIONS

It is very important to check sensitivity coefficients generated by TSUNAMI. The TSUNAMI-3D results can vary significantly depending on how the TSUNAMI input parameters are used and the accuracy of the modeling techniques used in cross-section generation and in the criticality calculations. The TSUNAMI-3D calculation performs separate forward and adjoint calculations and then uses the results to calculate sensitivity coefficients. Further discussion is provided in Section 4. Sensitivity coefficient results may be checked by performing DP calculations. In general, these calculations involve performing additional criticality calculations in which some target mixture or nuclide is manually varied about its nominal value and the results are used to manually calculate the sensitivity coefficients. The DP calculation of sensitivity coefficients provides only the integrated sensitivity coefficient (i.e., sum over all energy groups and reactions). It does not provide sensitivities as a function of energy or nuclear reaction (e.g., neutron scatter or neutron capture). DP calculations should be performed to check the TSUNAMI-3D results for both the application-specific models and the critical experiments used to support determination of an upper subcritical limit.

The DP method may use the values of k_{eff} from three criticality calculations to calculate a sensitivity coefficient. In addition to the nominal case, two additional calculations are performed with the composition of the material or nuclide of interest varied by plus and minus a few percent around the nominal value. The sensitivity coefficient may be calculated for a nuclide, mixture, or region using the following equation:

$$s = \frac{(k_1 - k_2)/k_{nominal}}{(\rho_1 - \rho_2)/\rho_{nominal}} \tag{1}$$

where ρ_1 and ρ_2 are the perturbed values of the density of a nuclide, mixture, or region around the nominal density and k_1, k_2, and $k_{nominal}$ are the k_{eff} values calculated at the respective densities.

The uncertainty in the sensitivity coefficient may be calculated using the following equation:

$$\sigma_s = \frac{1}{k_{nominal}} * \left[\sigma_{k_1}^2 + \sigma_{k_2}^2 + \left(\frac{k_1 - k_2}{k_{nominal}} \right)^2 * \sigma_{k_{nominal}}^2 \right]^{0.5} * \frac{\rho_{nominal}}{|\rho_1 - \rho_2|} \tag{2}$$

where σ_{k_1}, σ_{k_2}, and $\sigma_{k_{nominal}}$ are the calculated Monte Carlo standard deviations associated with k_1, k_2, and $k_{nominal}$.

The DP calculations are used to verify that the TSUNAMI-3D model adequately resolves the forward and adjoint flux solutions as a function of position and angle. The user may choose to perform DP calculations for all nuclides and mixtures. However, experience suggests that this is not necessary, because the same flux solution is typically used for many nuclides in the same region of the model. For a typical critical experiment, it is usually adequate to perform DP calculations for the primary fissile nuclide, the primary absorber in the fissionable material, and the primary moderating nuclide in moderated systems. Other DP calculations may be performed at the user's discretion as warranted by conditions of the specific model.

After 40 GWd/MTU of burnup, the GBC-32 cask model has both uranium and plutonium. The ^{235}U distribution, initially uniform axially, is depleted the most near the middle of the assembly and the least near the top. The plutonium is generated during power operation by neutron capture, primarily in ^{238}U. Consequently, the plutonium grows in with burnup and its distribution peaks near the middle and is lower at the ends of the assembly. Because the uranium and plutonium distributions have a different shape, DP calculations were performed for ^{235}U and ^{239}Pu to verify the accuracy of the sensitivity calculations for both nuclides. To generate accurate sensitivity coefficients, the flux solution must be resolved spatially such that the variation of the flux within a single region or mesh interval is minimized. Also, the order of the flux moments must be sufficient to capture any anisotropy of the flux solution, such as would occur near a vacuum boundary or strong absorber. The cask is modeled as flooded, so DP calculations were performed for the primary moderator, ^{1}H. Because the cask design includes Boral plates around each assembly, DP calculations were performed for ^{10}B. In summary, DP calculations were performed for ^{235}U, ^{239}Pu, ^{1}H, and ^{10}B.

Another issue to be considered is the width of the variation around the nominal densities for each material (ρ_1 and ρ_2) in Eq. 1. If too narrow a delta is used, the DP sensitivity coefficient may be driven more by the statistical variation in k_{eff} between the high- and low-density calculations than by the actual sensitivity. In general, the high-density and low-density criticality calculations should be about 10 standard deviations apart. If too large a delta is used, the DP sensitivity coefficient may miss some local nonlinear behavior of k_{eff} as a function of density. For example, if just enough ^{10}B is included in the cask design to effectively absorb all thermal neutrons entering the Boral plates, adding additional ^{10}B will have little effect on the system k_{eff}. Removal of ^{10}B from this same system may result in a more significant change in k_{eff}. Near this optimal ^{10}B density, DP calculations may not yield a sensitivity coefficient that is consistent with the data generated by TSUNAMI-3D. Trends of k_{eff} with changing density may be examined to determine if the DP-calculated sensitivity coefficient is affected by local nonlinear variation.

An alternative method for DP calculation of sensitivity coefficients is to perform k_{eff} calculations for several points within a range of densities (e.g., $\pm$10%) around the nominal density. The analyst may then normalize the calculated values of k_{eff} by dividing each k_{eff} by the nominal k_{eff} and normalize the densities by dividing each density by the density for the nominal case. A plot of the normalized k_{eff} as a function of the normalized density may be used to verify that the function behavior is linear in the vicinity of the nominal density. A linear least-squares fit of the data may be used to calculate the slope of the data and the standard error of the slope. This slope is the DP sensitivity coefficient. If the behavior is not linear, the approximate slope of the nonlinear curve in the vicinity of the nominal density may still be used to confirm the sensitivity coefficient generated by TSUNAMI-3D.

Some of the results from the DP calculations for the GBC-32 cask with W17×17OFA fuel burned to 40 GWd/MTU are presented in Table I. The DP results were obtained using a linear least-squares fit to several data points over a range of 90 to 110% of the nominal densities.

Table I. Direct perturbation calculation results

Nuclide or mixture	Sensitivity coefficient $(dk/k)/(d\rho/\rho)$
^{1}H	0.2490 ± 0.0049
^{10}B	-0.0312 ± 0.0007
^{235}U	0.1773 ± 0.0018
^{239}Pu	0.1118 ± 0.0009

The TSUNAMI-3D results should be statistically close to the DP results. If this is not the case, the user should examine the DP calculations and the TSUNAMI-3D model to resolve the differences.

4 TSUNAMI-3D MODEL

The input requirements for TSUNAMI-3D are very similar to those of the CSAS25 analysis sequence, which uses KENO V.a to perform criticality calculations. In addition to the normal CSAS25 model inputs, accurate TSUNAMI-3D modeling involves selecting the appropriate TSUNAMI input parameters and ensuring that the cross-section model is consistent with the geometry model. This section provides a discussion of the importance of consistent cross-section modeling as well as a discussion of TSUNAMI input parameters.

TSUNAMI-3D calculates total and partial sensitivity coefficients for various neutron interactions with each nuclide in each region. In some cases, these sensitivity coefficients may be further broken down into explicit and implicit components. The explicit component results from the sensitivity of k_{eff} to variation of the resonance self-shielded macroscopic cross section. The implicit component results from cross-section adjustments in the resonance self-shielding calculations. For example, the explicit sensitivity of hydrogen in the moderator around a fuel pin results directly from the sensitivity of k_{eff} to changes in the hydrogen cross section. The implicit sensitivity includes the effects of the sensitivity of the fuel macroscopic cross sections to changes in the moderator cross sections. The implicit component is calculated using derivatives produced during the problem-dependent cross-section processing.

4.1 Problem-Dependent Cross-Section Processing and Use

Erroneous implicit sensitivity coefficients may result if the cross-section model (e.g., lattice cell, multiregion, or infinite homogeneous) is not consistent with the way the material is used in the criticality model. The GBC-32 model has 18 axial fuel zones that at 40 GWd/MTU burnup, have significantly different fuel-region compositions. A separate lattice-cell cross-section model is run for each of the 18 axial zones. Thus, the derivatives needed to calculate the implicit sensitivity for hydrogen are available for all 18 zones. The impact of hydrogen cross-section variation on the fuel resonance calculations varies in these 18 zones. Consequently, the implicit contribution to the hydrogen sensitivity coefficient varies. If the criticality model does not use the same mixture numbers in the same places as the cross-section model, the wrong derivatives will be used to calculate the implicit contributions. For the GBC-32 model, a fuel rod could be modeled in the criticality calculation as a stack of 18 fuel regions enclosed by a single clad and a single moderator region. Because the cross-section model included 18 separate lattice-cell models, each with unique fuel, clad, and moderator mixture numbers, the variation of the derivatives with axial location would be discarded, because 17 of the 18 water and clad mixtures would not be used in the criticality model. The accurate criticality model for the GBC-32 fuel rods is formed by stacking 18 individual fuel rod segments, complete with clad and moderator, using the mixture numbers from the cross-section model. Thus, the correct implicit contributions will be calculated for each layer.

4.2 TSUNAMI-3D Options

The TSUNAMI-3D sequence uses forward and adjoint solutions, together with cross-section data and the derivatives used to calculate implicit sensitivities. Depending upon the TSUNAMI input options used, the amount of data being manipulated for a large model may become too large for many computing platforms. Decreasing the mesh size by a factor of 2 increases the memory required by a factor of 8. Additionally, the hard drive space requirements for the SCALE temporary directory may become quite large. In general, models should be set up as simply as possible to minimize computer memory and hard drive space requirements. The GBC-32 work reported in this paper utilized development versions of the TSUNAMI-3D programs and required more than 5 GB of RAM and about 10 GB of hard drive space to run. The simpler models more typically encountered in criticality safety can be accurately modeled with only a few hundred megabytes of RAM and hard drive space.

The selection of TSUNAMI-3D input parameters can significantly affect the results and computer resource requirements. Descriptions of the input options and variables are provided in the TSUNAMI-3D manual. For small, simple systems not containing strong absorbers, the defaults provided by the TSUNAMI-3D sequence will usually produce accurate sensitivity coefficients. However, the input options provided do enable the user to get accurate results for more complicated systems.

The TSUNAMI-3D user must check the final k_{eff} values for the forward and adjoint calculations to ensure that the same eigenvalue was obtained for both solutions. The k_{eff} values should not differ by more than 1% $\Delta k/k$. If they do, the user should examine the forward calculation to ensure that the fission source term is well converged. If convergence is questionable, standard methods for improving convergence should be used. If the forward calculation is well converged, the ***apg*** parameter may be used to increase the number of neutrons per generation in the adjoint calculation. For thermal systems, the default ***apg*** value, which is 3 times the ***npg*** value, should be adequate. For fast and intermediate spectrum systems, it may be necessary to use an ***apg*** value that is 10 times the ***npg*** value. Because of the nature of the adjoint calculations, it is not unusual for such calculations to fail the normality tests.

In addition to obtaining similar k_{eff} values for both forward and adjoint calculations, the user needs to verify that the DP calculations agree with the TSUNAMI-3D calculations. If the sensitivity coefficients do not agree, the TSUNAMI-3D input parameters may be modified to improve agreement.

Frequently, the most effective approach to obtaining adequate spatial resolution of the flux, which leads to accurate sensitivity coefficients, is to use the mesh flux accumulator. The mesh option may be turned on (i.e., ***mfx*** = yes) and the mesh size then specified (e.g., ***msh*** = 10). When the mesh option is used, the angular flux distributions and/or flux moments are accumulated for each region within each mesh rather than for each geometric region. Typically, the finer the mesh the more accurate the answer will be. However, the memory requirements for the TSUNAMI-3D run will increase proportionally with the total number of mesh. If the size of the mesh is cut in half, the memory requirements increase by a factor of 2^3. Due to computer memory limitations, in some models it may not be possible to use a sufficiently small mesh to get acceptable answers. For the GBC-32 cask model, using a mesh size no larger than 9 cm was the most important factor in obtaining accurate results.

Another potentially effective tool is to use coordinate transformation when accumulating flux moments and/or angular fluxes. This technique is generally most useful when the model has large regions and the mesh flux accumulator is not used. Several options are described in the manual for specifying various locations to be used as the origin for the purpose of flux moment calculation. The coordinate transform is turned on by setting the ***tfm*** variable to "true." The default transform origin is calculated as the center of the fissionable material regions. Oftentimes, this will be acceptable. At other times, this may place the origin in a very uninteresting part of the problem. In some calculations of the GBC-32 model, the transform origin was set near the horizontal center of the cask but was located vertically such that the origin was near the peak axial fission density, which occurred at about 20 cm below the top of the fuel. This is accomplished by using the ***center*** modifier in the geometry input.

The TSUNAMI-3D user has a choice between accumulating angular-dependent fluxes or accumulating flux moments with the ***nqd*** and ***pnm*** options, respectively. In general, accumulating angular fluxes will run faster than accumulating flux moments. This is true because the calculation of flux moments through a spherical harmonics expansion occurs only after the forward and adjoint transport calculations are completed. When the flux moments are accumulated, they are calculated with a spherical harmonics expansion for each particle track throughout the Monte Carlo calculation. The drawback is that accumulating angular fluxes with significant angular detail requires more computer memory. For example, if an S_{16} quadrature (***nqd*** = 16) is used, the 4π of space is divided into 288 solid angles and an independent flux solution will be generated for each angle. Angular flux distributions are generated for every KENO region (i.e., pellet, gap, clad, and moderator for each fuel rod), and these regions may be further subdivided if the mesh flux accumulator is used.

The flux moments may be calculated and accumulated with varying levels of angular detail. The order of the flux moment angular expansion may vary from zero, scalar flux, through a third-order ***(pnm*** = 3) expansion. Note that if both ***nqd*** and ***pnm*** are specified, both angular fluxes and flux moments are accumulated, increasing both memory and hard drive space requirements and the sensitivity coefficients are calculated using only the accumulated angular fluxes.

5 RESULTS

Selected GBC-32 TSUNAMI-3D sensitivity coefficient results are presented in Table II for the GBC-32 cask loaded with 32 Westinghouse 4 wt % ^{235}U 17 × 17 assemblies burned to 40 GWd/MTU and fully flooded. The sensitivity coefficients presented in the table represent the sensitivity of k_{eff} with respect to the total cross section for the given nuclide summed over all energy groups and all occurrences of the given nuclide in the model.

A series of calculations were performed with an 11.9-cm mesh (***mfx*** = yes, ***msh*** **=** 11.9) with first-, second-, and third-order flux moment expansions (***pnm*** = *1, 2, and 3*) and three options for the coordinate transform: no transform (***tfm*** = no), transform from the center of the fissile material (default) and transform from the location of the peak fission density (***tfm*** = yes and use of ***center*** in geometry input). The 11.9-cm mesh interval was selected because it is approximately one-half the width of a fuel assembly.

The coordinate transformation for flux moment calculations appears to have little effect on the flooded GBC-32 cask model. This finding is not surprising, because much of the model is segmented into many fairly small regions. The transform is generally most effective in models containing large regions. In the case where a fine computational mesh is used, the simplest option is typically to turn off the coordinate transform. Turning off the transform will reduce the run time.

For ^{235}U and ^{239}Pu sensitivity coefficients, the TSUNAMI-3D results agree reasonably well with the DP predictions. For nine cases with the 11.9-cm mesh, the sensitivity results are essentially unchanged with the various options for order of the angular moment expansion or choice of coordinate transform. For fissile nuclides, the sensitivity coefficients are largely derived from the scalar fluxes, which are not affected by these options.

For ^{1}H, the TSUNAMI-3D results are approximately 17% lower than the DP values and have large standard deviations. The sensitivity results vary by less than 2% according to order of the angular moment expansion and are essentially unchanged with the various options for the transform. The complexity of this model makes it difficult to obtain good statistics for all regions containing hydrogen. The TSUNAMI-3D results for ^{1}H do agree statistically with the DP results, but the discrepancies in the mean values could indicate that further model refinement is required for better agreement.

For ^{10}B, the TSUNAMI-3D results are 10 to 25% lower than the DP values. The sensitivity coefficients vary by 15% according to the order of the angular moment expansion but are unchanged by the transform options. The ^{10}B is present in thin panels between and around each fuel assembly. Thus, it is not surprising that the neutron flux in the thin panels has a strong angular dependence, which is more accurately resolved with a higher-order expansion. From the data, it is clear that second-order moment expansion is better than first order. However, it is not clear that third-order flux moment expansion is better than second order.

To investigate improvements to the series of calculations with the 11.9-cm mesh, a calculation was performed with 9-cm mesh (***mfx*** = yes, ***msh*** = 9), first-order flux moments (***pnm*** = 1), and the default transform. For this case, the agreement with DP for nuclides was improved relative to the corresponding 11.9-cm mesh calculation with first-order moments and the default transform. The 17% discrepancy for ^{1}H was reduced to 11%, and the 23% discrepancy for ^{10}B was reduced to 12%. Had this calculation been performed with a

Table II. TSUNAMI-3D sensitivity coefficient {(dk/k)/(dρ/ρ)} results for GBC-32

Direct perturbation results (S_{DP}) →					^{235}U	std dev	^{239}Pu	std dev	^{1}H	std dev	^{10}B	std dev	Figure of merit = $\sum_{nuc} \left\| S_{TSU3D} - S_{DP} \right\|$
					0.1773	**0.0018**	**0.1118**	**0.0009**	**0.2490**	**0.0049**	**−0.0312**	**0.0007**	
pnm[a]	**msh[b]**	**nqd[c]**	**tfm[d]**	**origin[e]**	**TSUNAMI-3D option-specific sensitivity coefficient (S_{TSU3D}) results**								
1	11.9		no		0.1849	0.0024	0.1264	0.0015	0.2080	0.0949	−0.0240	0.0002	0.070
2	11.9		no		0.1853	0.0016	0.1266	0.0016	0.2049	0.0972	−0.0283	0.0002	0.070
3	11.9		no		0.1853	0.0017	0.1266	0.0017	0.2056	0.0998	−0.0281	0.0003	0.069
1	11.9		yes	Default	0.1849	0.0024	0.1264	0.0015	0.2080	0.0949	−0.0240	0.0002	0.070
2	11.9		yes	Default	0.1853	0.0025	0.1266	0.0016	0.2049	0.0972	−0.0283	0.0002	0.070
3	11.9		yes	Default	0.1853	0.0026	0.1266	0.0017	0.2057	0.0998	−0.0281	0.0003	0.069
1	11.9		yes	peak fd[f]	0.1849	0.0024	0.1264	0.0015	0.2080	0.0949	−0.0240	0.0002	0.070
2	11.9		yes	peak fd	0.1851	0.0028	0.1267	0.0020	0.2072	0.1048	−0.0289	0.0004	0.067
3	11.9		yes	peak fd	0.1853	0.0026	0.1266	0.0017	0.2056	0.0998	−0.0281	0.0003	0.069
1	9		yes	Default	0.1824	0.0006	0.1160	0.0004	0.2214	0.0242	−0.0272	0.0001	0.041
	18	2	no		0.1839	0.0029	0.1256	0.0019	0.2374	0.1150	−0.0254	0.0003	0.038[g]
	18	4	no		0.1840	0.0029	0.1257	0.0019	0.1898	0.1125	−0.0311	0.0003	0.080
	18	6	no		0.1841	0.0029	0.1257	0.0019	0.1912	0.1123	−0.0323	0.0003	0.080

[a]pnm = order of flux moment expansion.
[b]msh = mesh length (cm) used in each direction.
[c]nqd = quadrature order for angular flux tallies.
[d]tfm = logical flag to perform coordinate transformation in accumulating flux moments and angular fluxes.
[e]Origin is the origin to be used in the coordinate transformation. The default is the center of the fissionable material.
[f]Axial location of peak fission density. This occurs about 20 cm below the top of the fuel.
[g]The data for this case are suspect. Lower-order quadrature should not produce better results than higher-order quadrature.

third-order flux moment, the ^{10}B results should have been further improved. However, the storage requirements to accumulate the higher-order spherical harmonics expansion would have been increased by a factor of 5.

The use of the angular flux accumulator for this problem was also investigated. However, due to the large number of angular solutions that must be stored for each mesh interval, the mesh size was limited to 18 cm and S_2, S_4, and S_6 angular quadratures were investigated. One aberration to consider is the apparent good prediction for ^1H provided by ***nqd*** = 2 (one angle per octant). This result is suspect because increasing ***nqd*** to higher values (more angular detail) produced larger deviations from the DP results. It is likely that the apparent good results for ***nqd*** = 2 are due to coincidental cancellation of errors. Otherwise, with increasing quadrature order, the ^{235}U and ^{239}Pu results are constant, and the ^{10}B results improve relative to the DP results.

The results for the finest mesh (***msh*** = 9) and first-order flux moments (***pnm*** = 1) produced the best overall results, as demonstrated by the figure of merit in Table II. The figure of merit is the sum of the absolute values of the differences between the DP results and the TSUNAMI-3D results for each nuclide. It is recommended that for models similar to the GBC-32 cask (e.g., large SNF storage arrays utilizing neutron poison panels), the smallest mesh possible should be used. The use of first-order flux moments instead of second- or third-order expansions or angular flux accumulation will reduce the memory requirements for flux storage and allow for the use of a finer mesh. Follow-on work, not reported in this paper, indicates that no additional accuracy is obtained below a specific model-dependent mesh size. For the GBC-32 cask model, reducing the mesh size below 9 cm produced no obvious improvement. Once this minimum mesh size is identified, other options such as increasing ***pnm*** or ***nqd*** should be explored to gain further improvement.

Although it may be difficult to obtain excellent agreement between DP calculations and TSUNAMI-3D results for hydrogen for large and complex models (e.g., the GBC-32 cask loaded with SNF), excellent agreement has been achieved for less complex models. A detailed explanation of the use of TSUNAMI-3D for a critical experiment is documented in reference 5.

6 COMPARISON WITH CRITICAL EXPERIMENTS

One of the primary objectives for performing sensitivity analysis is to enable comparison of criticality safety analysis calculations with benchmark critical experiments [6]. Traditionally, an analyst would identify a set of critical experiments that were, in the analyst's opinion, similar to a model of normal and/or upset conditions associated with a fissionable material operation. TSUNAMI-3D permits a more detailed comparison of various aspects of calculational models. As part of a larger project, work is ongoing to establish bases for taking credit for some fission products in burnup credit for transport of SNF.

Some critical experiments have been performed and others are planned that include some of the highest-reactivity-worth fission products. TSUNAMI-3D has been used to generate sensitivity coefficients for critical experiments that include ^{149}Sm, ^{103}Rh, and ^{155}Gd. This work is ongoing and will be reported at a later date. Figures 1 and 2 show energy-dependent sensitivity coefficient profiles for ^{149}Sm and ^{103}Rh from two critical experiment models and from the GBC-32 cask model. In the legend for these figures, the "a" value is the sensitivity coefficient and the "osc" value is the oppositely signed component of the sensitivity coefficient. For example, in Figure 1 the sensitivity coefficient for the total macroscopic cross section for ^{149}Sm is

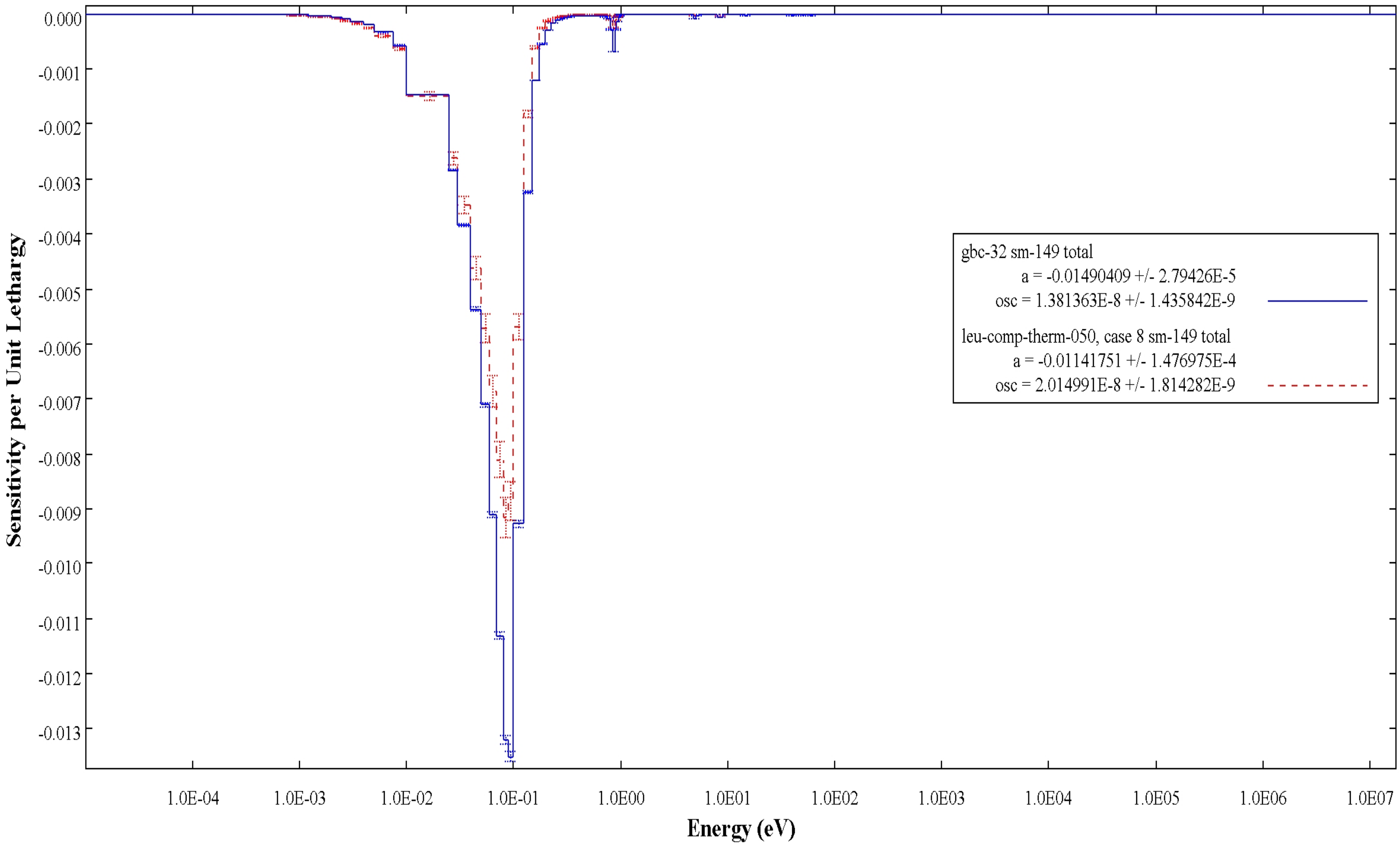

Figure 1. Energy-dependent sensitivity profile for ^{149}Sm in a fission product critical experiment model and in the GBC-32 burnup credit cask model.

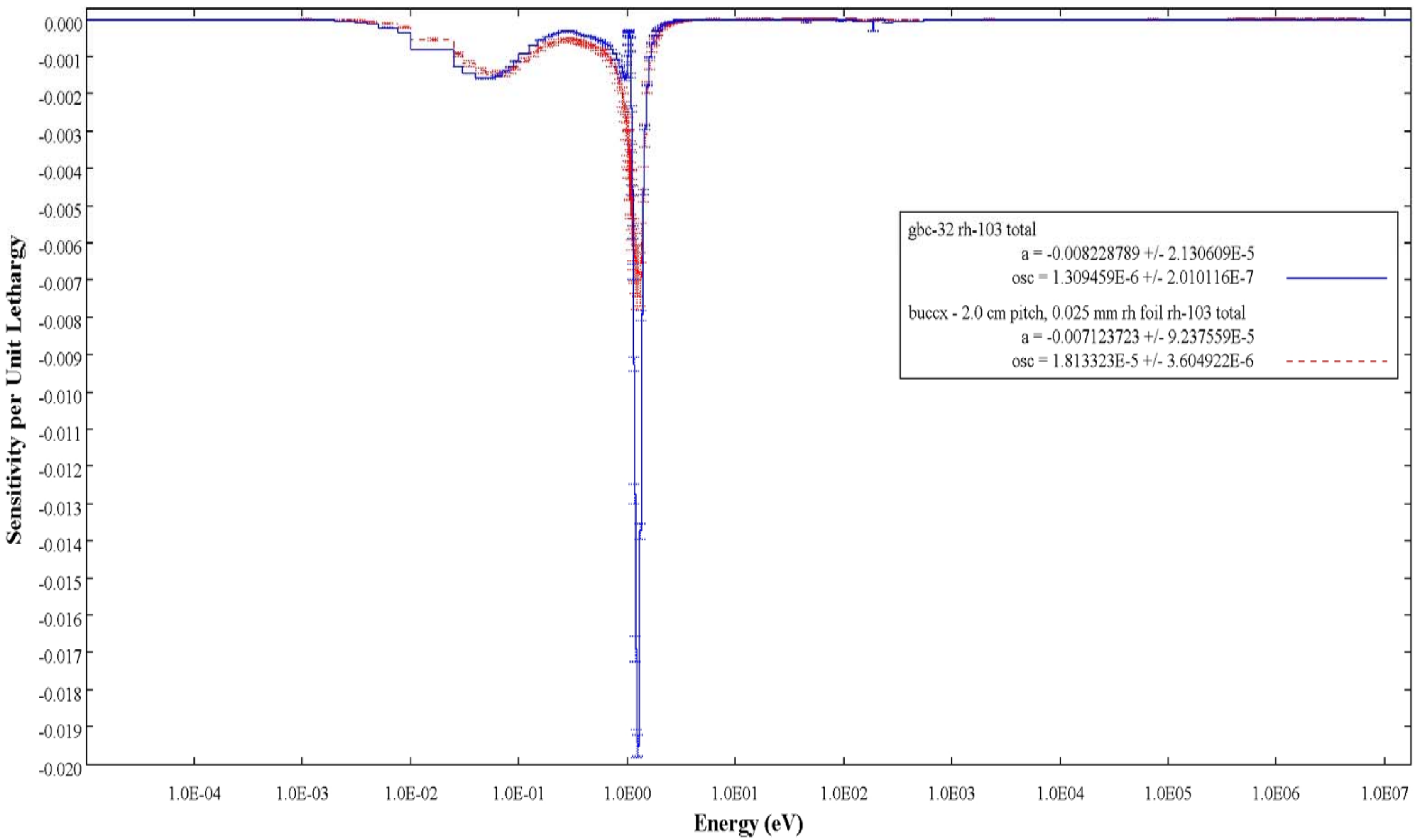

Figure 2. Energy-dependent sensitivity profile for ^{103}Rh in a fission product critical experiment model and in the GBC-32 burnup credit cask model.

$-0.01490409 \pm 2.79426 \times 10^{-5}$ (δk/k)/(δΣ/Σ). The total positive contribution to this value is $1.381363 \times 10^{-8} \pm 1.435842 \times 10^{-9}$ (δk/k)/(δΣ/Σ). Qualitatively, the profiles from these critical experiments show significant similarity to the profiles from the GBC-32 burnup credit model. The GBC-32 model is more sensitive to the presence of these two fission products than these two critical experiment models. TSUNAMI-3D could be used in this way as another tool for the design of future critical experiments.

The SCALE TSUNAMI-IP code, first distributed publicly with SCALE 5.0, is used to perform a detailed comparison of the sensitivity coefficient information from different models and will be used to quantitatively determine if the fission product critical experiments are sufficiently similar to the GBC-32 burnup credit model to provide adequate validation. This work is ongoing and will be reported in the future.

7 CONCLUSIONS

This paper describes the creation of a TSUNAMI-3D model for a generic burnup credit cask. Guidance and recommendations were provided for performing DP calculations to check TSUNAMI-3D results and for selection of TSUNAMI-3D modeling techniques and input parameters. Results from careful DP calculations provide an essential check on the accuracy of TSUNAMI-3D sensitivity coefficients. Of the various options tested, the best TSUNAMI-3D GBC-32 cask model was produced by using a 9-cm mesh size (***msh*** = 9), accumulating flux moments using a second-order expansion (***pnm*** = 2), and turning the coordinate transformation setting off (***tfm*** = no). Sensitivity coefficient results for the GBC-32 burnup credit cask were presented. Sensitivity profiles generated for ^{149}Sm and ^{103}Rh for two critical experiments were qualitatively compared with sensitivity profiles for the GBC-32 burnup credit cask.

8 ACKNOWLEDGMENT

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