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Applications of the TSUNAMI Sensitivity and Uncertainty Analysis Methodology

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The TSUNAMI sensitivity and uncertainty analysis tools under development for the SCALE code system have recently been applied in four criticality safety studies. TSUNAMI is used to identify applicable benchmark experiments for criticality code validation, assist in the design of new critical experiments for a particular need, reevaluate previously computed computational biases, and assess the validation coverage and propose a penalty for noncoverage for a specific application.

***KEYWORDS:** Sensitivity and uncertainty analysis, area of applicability*

1. Introduction

Several practical applications of Tools for Sensitivity and UNcertainty Analysis Methodology Implementation (TSUNAMI)[1,2] under development for the SCALE[3] code system have recently demonstrated the usefulness of this analysis approach. TSUNAMI consists of a number of sensitivity and uncertainty analysis tools that were developed primarily to assess the area of applicability of critical experiments for use in criticality code validations. Sensitivity coefficients produced by the TSUNAMI sensitivity analysis sequences predict the relative changes in a system's multiplication factor, k_{eff}, due to relative changes in the neutron cross-section data. TSUNAMI generates sensitivity coefficients from a one-dimensional deterministic neutron transport analysis or a three-dimensional (3-D) Monte Carlo neutron transport analysis. Uncertainties in the cross-section data are propagated to an uncertainty in k_{eff} via the sensitivity coefficients.

Integral indices, developed for TSUNAMI, give a quantitative measure of the similarity of a benchmark experiment and a design system based on the differential sensitivity and/or uncertainty data for each reaction of each nuclide on an energy-dependent basis. If the design system is assessed as similar to the benchmark experiment, it is deemed that the design system falls within the area of applicability of the experiment. Further TSUNAMI analyses assess validation coverage for a particular reaction of a given nuclide by a benchmark experiment based on the sensitivity data. Three integral indices, c_k, E_{sum}, and g, are used in this paper to evaluate system similarity with sensitivity and uncertainty data (c_k),[2] evaluate system similarity only with sensitivity data (E_{sum}),[2] and evaluate benchmark coverage for a specific nuclide and reaction with sensitivity data (g).[4]

Four recent studies have demonstrated some uses of the TSUNAMI techniques. TSUNAMI was used to select experiments for criticality code validation for a weapons-grade (WG) mixed-oxide (MOX) fuel fabrication facility application, assist in the design of new critical experiments intended to validate UO_2 light-water-reactor (LWR) fuel with enrichments >5 wt % in ^{235}U, assess subcritical limits as an alternative to traditional trending parameters for TRUPACT and HalfPACT shipping packages, and assess validation coverage for ^{10}B capture for LWR fuel shipping packages that are poisoned with boron. Each of these studies is described in subsequent sections.

2. Use of TSUNAMI in the Selection of Experiments for Criticality Code Validation

TSUNAMI techniques were used to assess the applicability of existing benchmark experiments for the criticality code validation of a WG-MOX fuel fabrication facility.[5] In this study, the applicability of 318 critical experiments to the validation of a particular MOX powder design configuration was evaluated. The system considered is a critical sphere of MOX powder with a density of 5.5 g/ml and 5 wt % H_2O. The MOC consists of 22 wt % WG-PuO_2 (96 wt % ^{239}Pu, 4 wt % ^{240}Pu) and 78 wt % depleted UO_2 (0.3 wt % ^{235}U, 99.7 wt % ^{238}U). A 60-cm-thick depleted uranium reflector surrounds the MOX sphere. This system exhibits an H/(U+Pu) atomic ratio of 1.58 and an energy of average lethargy causing fission (EALF) value of 3751 eV.

Sensitivity coefficients for the MOX application and each of the 318 benchmark experiments were generated with the TSUNAMI sensitivity analysis sequences of SCALE. The sensitivity data were then processed with cross-section covariance data to form

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correlation coefficients that give a measure of the common uncertainty in the computed k_{eff} values between the MOX application and a given benchmark experiment. The k_{eff} correlation coefficient, referred to as c_k, has a range of values between 0 and 1, where 0 indicates that the systems are not similar and 1 indicates that the systems are fully correlated. In this study, a c_k value of 0.8 or higher between the MOX system and a benchmark experiment indicates that the experiment is similar enough to the MOX application to be useful in the criticality code validation.

For this MOX application, 53 of the 318 benchmark experiments exceed the 0.8 criterion for c_k. Of these, 18 values exceed 0.9, indicating a high degree of similarity. Of the 53 experiments with c_k values exceeding 0.8, 33 are MOX fueled and the remaining 20 are plutonium fueled. The matching systems exhibited EALF values of approximately 40 eV, whereas the EALF of this application is nearly 4000 eV. Thus, the TSUNAMI methods have identified applicable experiments that might not have been selected through traditional means.

The selection by the TSUNAMI methods of certain experiments as applicable to the MOX application can be explained through examination of the sensitivity data on which the correlation coefficients are based. Two experiments examined in this study, experiment 1 from NSE-55 table 4 [NSE55T4-01][6] and experiment 4 from NSE-55 table 5 [NSE55T5-04], exhibit EALF values of 0.143 and 41.0 eV, respectively. Based on EALF alone, these experiments would not be selected for the validation of a MOX application with an EALF value of 3751 eV. However, the TSUNAMI methods provide a more rigorous analysis. The energy-dependent sensitivity profiles for ^{239}Pu fission for the MOX application and benchmark experiments NSE55T4-01 and NSE55T5-04 are shown in Fig. 1. The sensitivity of the MOX application is most significant in the fast energy region with some significant values in the thermal region. The peak values in the resonance region are also large, but their contribution to the integral of the sensitivity profile is limited by their small group widths. With the TSUNAMI methodology, the sensitivity profiles of the benchmark experiment for all significant nuclide reactions must sufficiently match those of the application over the entire energy range to demonstrate applicability. The sensitivity of NSE55T4-01 is strongly peaked in the thermal energy region, with almost no sensitivity in the fast region. Thus, NSE55T4-01 is a poor match for the MOX application, and when all nuclides are examined, a low c_k value of 0.51 results. Experiment NSE55T5-04 exhibits more sensitivity in the thermal region than does the MOX application but also exhibits significant sensitivity in the fast region, and a high c_k value of 0.91 is produced. Therefore, although the EALF value shows that the MOX application and NSE55T5-04 have different average parameters, the TSUNAMI methodology shows that the most significant areas of the application are, in fact, covered by the benchmark experiment. Furthermore, the TSUNAMI methodology confirms that experiment NSE55T4-01 is not applicable to the validation of the MOX application. For more information on this application of TSUNAMI, please see Ref. 5.

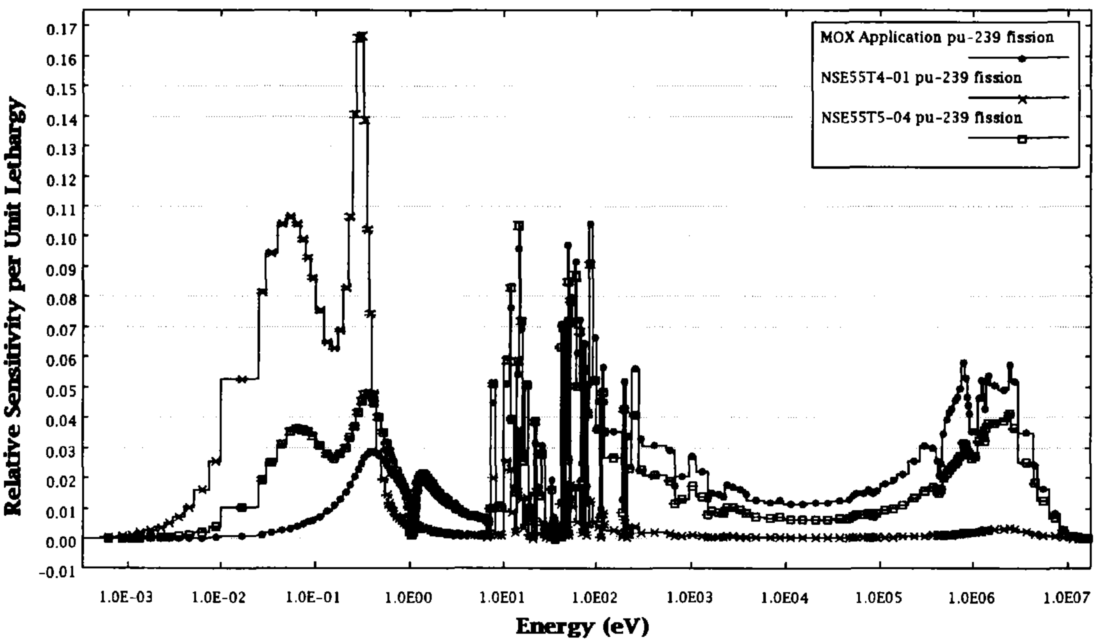

Fig. 1 Energy-dependent sensitivity profiles for ^{239}Pu fission for MOX application, experiment 4 from NSE-55 table 5 and experiment 1 from NSE-55 table 4.

3. Use of TSUNAMI in Critical Experiment Design

TSUNAMI methodology has been applied to optimize the design of new critical experiments.[7] This particular analysis assists in ensuring that an experimental series to be constructed of lattices of UO_2 fuel rods with an enrichment of 6.93 wt % in ^{235}U will provide validation coverage for prototypic UO_2 commercial reactor fuel with enrichments between 5 and 10 wt % ^{235}U.

3.1 Conceptual Experiment Design

Two conceptual experiment designs, constrained by available materials and facilities, were proposed for the series of critical assemblies desired in this project. In each design, the fuel consists of sintered-UO_2 pellets with a U enrichment of 6.93 wt % ^{235}U with an outer diameter of 0.526 cm and a density of 10.29 g/cm^3. The pellets are loaded in aluminum cladding with an outer diameter of 0.635 cm. The active fuel height is 50 cm and is fully flooded with borated water. For compatibility with commercial lattice-physics codes, the critical cores must be composed of symmetric square arrays of fuel rods. The first proposed experiment design is comprised of a square array of square-pitched fuel rods, requiring 1836 rods. The second design consists of the cruciform design of square-pitched fuel rods, requiring 1596 rods. Each conceptual geometrical design includes eight critical configurations with varying fuel-rod pitch, temperature (20 and 60°C), and absorber rods. Criticality is achieved by diluting soluble boron from the moderator. In each conceptual design, 4 of the 8 critical configurations contain 20 UO_2-Gd_2O_3 burnable poison (BP) rods, with 4 wt % Gd_2O_3, a ^{235}U enrichment of 4 wt %, and the same dimensions and cladding as the fuel rods.

3.2 Representative Commercial Fuel Designs

Representative fuel assemblies of widely used commercial power reactor fuels were selected for analysis in this study. The selected representative assemblies are not the result of a comprehensive review of all nuclear fuel designs that could eventually be produced with higher enrichments but are selected only to show trends in the data with regard to the applicability of the experimental data. Additional fuel designs may be considered in future analyses as needed.

Three commercial fuel designs were considered in this study: the Babcock and Wilcox (B&W) 15×15 fuel assembly, the Westinghouse 17×17 fuel assembly, and the General Electric (GE) 8×8 fuel assembly. Each of the commercial assemblies was modeled with ^{235}U enrichments of 4, 6, 7, and 10 wt %. Furthermore, each configuration was modeled under various conditions that could be encountered throughout the fuel cycle, excluding burnup. Each design was modeled at two temperatures. Shipping, storage, and initial core-loading conditions were simulated with models at 20°C. Average properties at operating conditions were modeled at higher temperatures, specific to each assembly type.

BP rods of UO_2-Gd_2O_3 were also considered in the commercial fuel models. The number of poison rods, when present, for each assembly type was as follows: B&W 15×15, 20 BPs; Westinghouse 17×17, 24 BPs; and GE 8×8, 8 BPs.

3.3 TSUNAMI Analysis

The TSUNAMI methodology was applied to determine which conceptual design experimental series was the most applicable to the commercial assemblies considered. Sensitivity data were generated for each conceptual design configuration and representative commercial assembly using the 3-D Monte Carlo sensitivity analysis sequence TSUNAMI-3D. Because cross-section covariance data for Gd are not available, the correlation coefficient c_k could not be used reliably for this analysis. The alternative integral parameter E_{sum} was used to assess the similarity of the experiment designs to the commercial assemblies based only on the sensitivity data. The parameter E_{sum} has the same limits as c_k, and in this study, an E_{sum} value of 0.8 or higher indicates that the experiment is similar enough to the application to be useful in its criticality code validation.

The numbers of the eight proposed critical configurations with E_{sum} exceeding 0.8 for each experimental series are shown in Tables 1 and 2 for the square-design experiments and the cruciform-design experiments, respectively. All eight of the square-design experiments exceed the 0.8 criteria for all low-temperature commercial assemblies studied, except for the 4.0 wt % enriched GE assembly. Some of the square-design experiments were applicable to the high-temperature assemblies. The results for the cruciform-design experiments show that fewer critical experiments are applicable to the low-temperature commercial assemblies and that almost none are applicable to the high-temperature assemblies.

Based on these results, and more detailed nuclide-reaction-specific analyses not presented here, the square-design experiments have been selected as the preferred design for the experimental series.

4. Use of TSUNAMI in Trending Analyses

TSUNAMI was applied to the criticality safety analysis of the TRUPACT-II and HalfPACT over-the-

Table 1 Numbers of the eight square-design experiments with $E_{sum} \geq 0.8$ in relation to commercial assemblies

		Low temperature		High temperature	
Enrichment	**Assembly**	**No BP**	**BP**	**No BP**	**BP**
4.0 wt %	GE		7		8
	B&W	8	8	6	2
	West.	8		8	7
6.0 wt %	GE		8		3
	B&W	8	8	2	0
	West.	8		5	1
7.0 wt %	GE		8		2
	B&W	8	8	0	0
	West.	8		5	1
10.0 wt %	GE		8		0
	B&W	8	8	0	0
	West.		8	0	0

Table 2 Numbers of the eight cruciform-design experiments $E_{sum} \geq 0.8$ in relation to commercial assemblies

		Low temperature		High temperature	
Enrichment	**Assembly**	**No BP**	**BP**	**No BP**	**BP**
4.0 wt %	GE		8		8
	B&W	7	7	0	0
	West.	7		4	0
6.0 wt %	GE		8		0
	B&W	6	7	0	0
	West.	7		0	0
7.0 wt %	GE		8		0
	B&W	5	6	0	0
	West.	7		0	0
10.0 wt %	GE		8		0
	B&W	2	4	0	0
	West.		5	0	0

road fissile material shipping containers.[8] When the TSUNAMI integral indices are used in place of H/^{239}Pu atomic ratios in trending analyses, a new subcritical limit is realized and the mass limits for the containers could potentially be increased by 7–20%.

The potential increase is due to the significant difference between historical computational bias trending methods and the use of the recently developed TSUNAMI integral parameter c_k. An excessive computational bias (i.e., nearly +0.04 in k_{eff}) was determined in the safety analysis report for the TRUPACT-II package[9] using classical trending for critical experiment–calculated biases with the hydrogen-to-fissile atom ratios (i.e., H/^{239}Pu). The use of the integral c_k parameter has demonstrated that a more realistic computational bias is on the order of about +0.015 in k_{eff}.

Figures 2–4 show some of the results of trending the calculated k_{eff} of critical experiments with the c_ks of particular TRUPACT-II payload containers. The linear fits of the computed benchmark $k_{eff,\ inf}$ values have been weighted by a cumulative normal distribution ranging from 1 at $c_k = 1.0$ to nearly 0.0 at $c_k = 0.0$ (assuming 5 standard deviations).

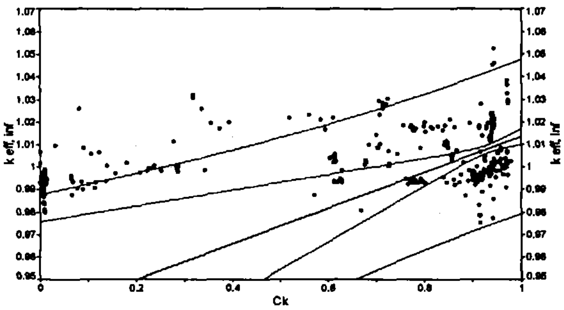

Fig. 2 Infinite array of TRUPACT-IIs with 55-gallon drums, $k_{eff,\ inf} = 0.9340 + 0.0797c_k$ (1.0137) with 99% confidence intervals.

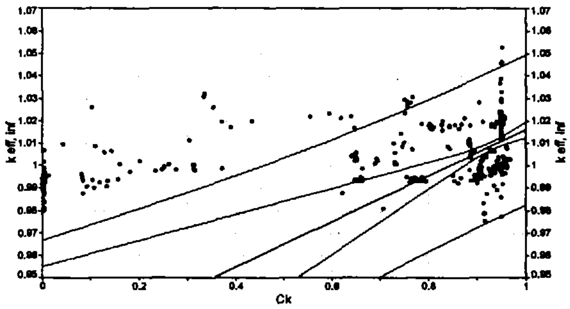

Fig. 3 Infinite array of TRUPACT-IIs with 6-in. pipe overpack container, $k_{eff,\ inf} = 0.9135 + 0.1016c_k$ (1.0151) with 99% confidence intervals.

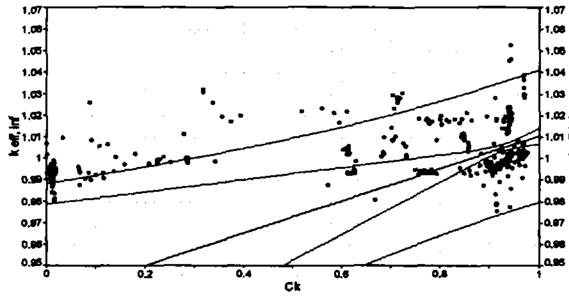

Fig. 4 Infinite array of TRUPACT-IIs with 12-in. pipe overpack container, $k_{eff,\ inf} = 0.9350 + 0.0756c_k$ (1.0106) with 99% confidence intervals.

5. Use of TSUNAMI in Assessment of Validation Coverage for a Specific Nuclide and Reaction

In another study, the TSUNAMI nuclide-reaction-specific tools were used to assess the validation coverage for boron capture in commercial shipping packages that utilize large amounts of boron to reduce reactivity.

The integral parameters E_{sum} and g were used to assess the area of applicability of numerous water-moderated low-enriched uranium (LEU) benchmarks for five application casks containing LWR fuel and high concentrations of ^{10}B. Some parameters of the nuclear fuel cask models, including the calculated EALF and the calculated ^{10}B capture sensitivity coefficients, are summarized in Table 3.

The E_{sum} values were computed for each experiment in relation to each cask application. The E_{sum} values, not shown for purposes of brevity, are quite high and demonstrate that most of the benchmarks are very similar to the cask models and are appropriate for use in criticality code validations. One exception is the GBC-32 cask, for which the largest E_{sum} value is only 0.63. However, the values of E_{sum} are strongly dominated by the ^{235}U fission and ^{1}H scattering reactions. Thus, these values are more indicative of the use of water-moderated LEU fuel in both the benchmarks and the cask models.

The nuclear fuel cask models were also analyzed with the nuclide-reaction-specific g parameter. This parameter assesses the benchmark coverage of a specific reaction of a specific nuclide based on the energy-dependent sensitivity data. As with the c_k and E_{sum} parameters, the range of g is 0 to 1, where 1 indicates complete coverage for the given reaction. The maximum g values for ^{10}B capture, and ^{235}U fission and ^{1}H scatter sensitivity coefficients along with the maximum g values for these nuclide-reaction pairs are listed in Table 4. As the g values in the table show, the benchmarks provide poor coverage for ^{1}H scatter for the GBC-32 cask. This is the reason the E_{sum} value for this cask is small. As the g values indicate, none of the benchmarks are as sensitive to ^{10}B capture across the entire energy range as any of the applications. The maximum g values for ^{235}U fission and ^{1}H scatter are much higher than the maximum g values for the ^{10}B capture, indicating that the benchmarks provide good coverage for ^{235}U fission and ^{1}H scatter but poor coverage for ^{10}B capture. Also, the applications are much more sensitive to ^{235}U fission and ^{1}H scatter than ^{10}B capture.

Finally, the calculated k_{eff} values for the application casks have been adjusted by applying a penalty for not having complete coverage by the benchmarks. Calculated k_{eff} values for the application casks, along with the adjusted k_{eff} values, are listed in Table 5. The adjusted k_{eff} is the calculated k_{eff} increased by a penalty value. This penalty is computed by multiplying the value of the portion of the application sensitivity that is not covered by any benchmarks by the uncertainty in the k_{eff} of the cask due to ^{10}B capture cross-section uncertainties. The penalty due to noncoverage of ^{10}B capture cross sections is small, with a maximum value of 0.8% in k_{eff}. Therefore, it was concluded that although sufficient benchmark experiments did not exist to provide coverage for all design scenarios, the potential impact of the noncoverage on the criticality safety of the shipping package was minimal.

The penalty due to noncoverage by the benchmarks (i.e., the penalty due to the application not being in the area of applicability of benchmarks completely) could be used as an additional subcritical margin in licensing calculations.

Table 3 Nuclear fuel cask model parameters

Cask	Calculated $k_{eff} \pm \sigma$	EALF (eV)	^{10}B Capture sensitivity	^{10}B Form	Total ^{10}B (kg)	^{10}B Surface density (at/cm^2)
MPC-24	0.9458 ± 0.0005	2.257E-01	-2.62E-02	Boral	~12	1.216E+21
MPC-68	0.9349 ± 0.0005	2.775E-01	-5.05E-02	Boral	~15	1.658E+21
GA-4	0.9221 ± 0.0005	4.572E-01	-2.38E-02	B_4C	~8	4.750E+22
GBC-32	0.8941 ± 0.0004	2.474E-01	-2.76E-02	Boral	~12	1.688E+21
OECD	1.1303 ± 0.0005	6.311E-02	-4.45E-02	Borated steel	~6	3.918E+20

Table 4 Sensitivity coefficients and maximum g values for all applications

Cask	Maximum g value for ^{10}B capture	^{235}U Fission sensitivity	^{1}H Scatter sensitivity	Maximum g value for ^{235}U fission	Maximum g value for ^{1}H scatter
MPC-24	0.79	0.325	0.253	0.97	0.93
MPC-68	0.46	0.344	0.214	0.93	0.84
GA-4	0.29	0.367	0.345	0.99	0.85
GBC-32	0.73	0.154	0.233	1.00	0.68
OECD	0.75	0.376	0.148	0.99	0.86

Table 5 Penalty assessments for noncoverage of ^{10}B captures

Cask	Calculated k_{eff}	^{10}B capture sensitivity that is not covered by any benchmark	Penalty in k_{eff} due to noncovered sensitivity for ^{10}B capture (%)	Adjusted k_{eff}
MPC-24	0.9458	-4.76E-04	0.04	0.9462
MPC-68	0.9349	-1.91E-02	0.31	0.9380
GA-4	0.9221	-1.69E-02	0.07	0.9228
GBC-32	0.8941	-1.65E-03	0.8	0.9021
OECD	1.1302	-5.73E-03	0.02	1.1304

6. Conclusions

This paper has demonstrated the use of the TSUNAMI techniques for four criticality safety applications. In each case, new information is realized through the use of the advanced analysis techniques. When properly applied, this new information could lead to the better utilization of existing critical experiments, optimization of new experiment designs, improved computational biases, and a better understanding of the processes that are important in nuclear designs.

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