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## **Application of Sensitivity and Uncertainty Analysis Methods to a Validation Study for Weapons-Grade Mixed-Oxide Fuel**

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# Application of Sensitivity and Uncertainty Analysis Methods to a Validation Study for Weapons-Grade Mixed-Oxide Fuel

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## Executive Summary

At the Oak Ridge National Laboratory (ORNL), sensitivity and uncertainty (S/U) analysis methods and a Generalized Linear Least-Squares Methodology (GLLSM) have been developed to quantitatively determine the similarity or lack thereof between critical benchmark experiments and an application of interest. The S/U and GLLSM methods provide a mathematical approach, which is less judgment based relative to traditional validation procedures, to assess system similarity and estimate the calculational bias and uncertainty for an application of interest. The objective of this paper is to gain experience with the S/U and GLLSM methods by revisiting a criticality safety evaluation and associated traditional validation for the shipment of weapons-grade (WG) MOX fuel in the MO-1 transportation package. In the original validation, critical experiments were selected based on a qualitative assessment of the MO-1 and MOX contents relative to the available experiments. Subsequently, traditional trending analyses were used to estimate the  $\Delta k$  bias and associated uncertainty. In this paper, the S/U and GLLSM procedures are used to re-evaluate the suite of critical experiments associated with the original MO-1 evaluation. Using the S/U procedures developed at ORNL, critical experiments that are similar to the undamaged and damaged MO-1 package are identified based on sensitivity and uncertainty analyses of the criticals and the MO-1 package configurations. Based on the trending analyses developed for the S/U and GLLSM procedures, the  $\Delta k$  bias and uncertainty for the most reactive MO-1 package configurations are estimated and used to calculate an upper subcritical limit (*USL*) for the MO-1 evaluation. The calculated bias and uncertainty from the S/U and GLLSM analyses lead to a calculational *USL* that supports the original validation study for the MO-1.

## I. Introduction

An integral part of a criticality safety analysis is the validation of the calculational method (i.e., computer code modeling approximations, and cross-section library) against applicable experimental data [1]. "Traditional" validation methods require the establishment of bias values based upon the use of benchmark experiments that are *judged* to be similar to the application of interest. Moreover, the traditional methods invariably rely upon the expert judgment of the nuclear analyst to establish the area of applicability for the validation. Current efforts at the Oak Ridge National Laboratory

(ORNL) have lead to the development of sensitivity and uncertainty (S/U) analysis methods and a Generalized Linear Least-Squares Methodology (GLLSM) that can be used to determine areas of applicability and subcritical margins for nuclear criticality safety applications [2]. The S/U and GLLSM methods provide a more rigorous and less judgment-based approach for performing validation studies. The details of the S/U and GLLSM methods are well documented [3, 8] and are not developed in this paper; however, brief descriptions of each method are presented to highlight the features of the S/U and GLLSM methods. The objective of this work is to gain experience in the use of the S/U and GLLSM methods by applying the analysis procedures to a validation for weapons-grade (WG) mixed-oxide (MOX) fuel.

## II. MOX Application

The application of interest stems from the Fissile Material Disposition Program (FMDP) which is tasked with implementing the Department of Energy (DOE) formal Record of Decision for the storage and disposition of surplus WG plutonium. One disposition option involves the irradiation of surplus plutonium as MOX fuel in existing light-water reactors (LWR). A crucial part of the MOX fuel disposition approach involves the transportation of MOX assemblies from the fuel fabrication facility to one or more existing commercial LWR sites. To fulfill the disposition objectives, the FMDP considered use of the MO-1 package [4], which was originally developed by Westinghouse, to transport lead-test MOX assemblies. The application for license revision of the MO-1 must include a criticality safety analysis of the package under various transport conditions.

A schematic diagram of the MO-1 package is provided in Figure 1. The external containment vessel or overpack consists of an inner and outer carbon-steel shell. The volume between the shells is filled with a shock and thermal insulating material consisting of rigid polyurethane foam ( $\rho = 8 \times 10^{-2}$  g/cc). The internal and external shells are separated into upper and lower sections of the package as shown in Figure 1. When assembled, the upper and lower sections form a rectangular box with a central separation plane. As shown in Figure 1, the internal support structure is composed of a carbon-steel strongback frame that can support a maximum of 2 fuel assemblies in the package. A 3.8 cm gap region is located between the two assembly locations, and a full-length 0.48 cm-thick borated SS304 plate is positioned on either side of the gap region to provide neutron absorption. During transport, the fuel assemblies are secured to the strongback by a series of 8 carbon-steel clamping frames that are located along the entire length of the assembly. The entire strongback support frame is attached to the inner shell of the MO-1 by 18 rubber shock absorbers that suspend the internals within the package and provide shock and vibration isolation for the fuel during transport.

At the time of the evaluation, only preliminary designs of the lead test MOX assemblies were available for consideration. For the purposes of this work, a 17×17 Westinghouse PWR fuel assembly is considered in the evaluation of the MO-1 transport package. The assembly consists of 264 fuel rods with 25 guide tubes arranged on a 1.26 cm pitch. Each fuel pin has a Zircaloy-4 cladding with an outer diameter of 0.9144 cm. The fuel pellet outer diameter is 0.7844 cm, and the length of the fuel region is 365.8 cm. The MOX fuel is 4.803 wt % plutonium (93.6 wt %  $^{239}\text{Pu}$ , 5.9 wt %  $^{240}\text{Pu}$ ,

0.4 wt %  $^{241}\text{Pu}$ , and 0.1 wt %  $^{242}\text{Pu}$ ). The uranium in the MOX fuel is depleted (i.e., 0.2 wt %  $^{235}\text{U}$  and 99.8 wt %  $^{238}\text{U}$ ). Additional details for the fuel assembly are provided in Ref. [4].

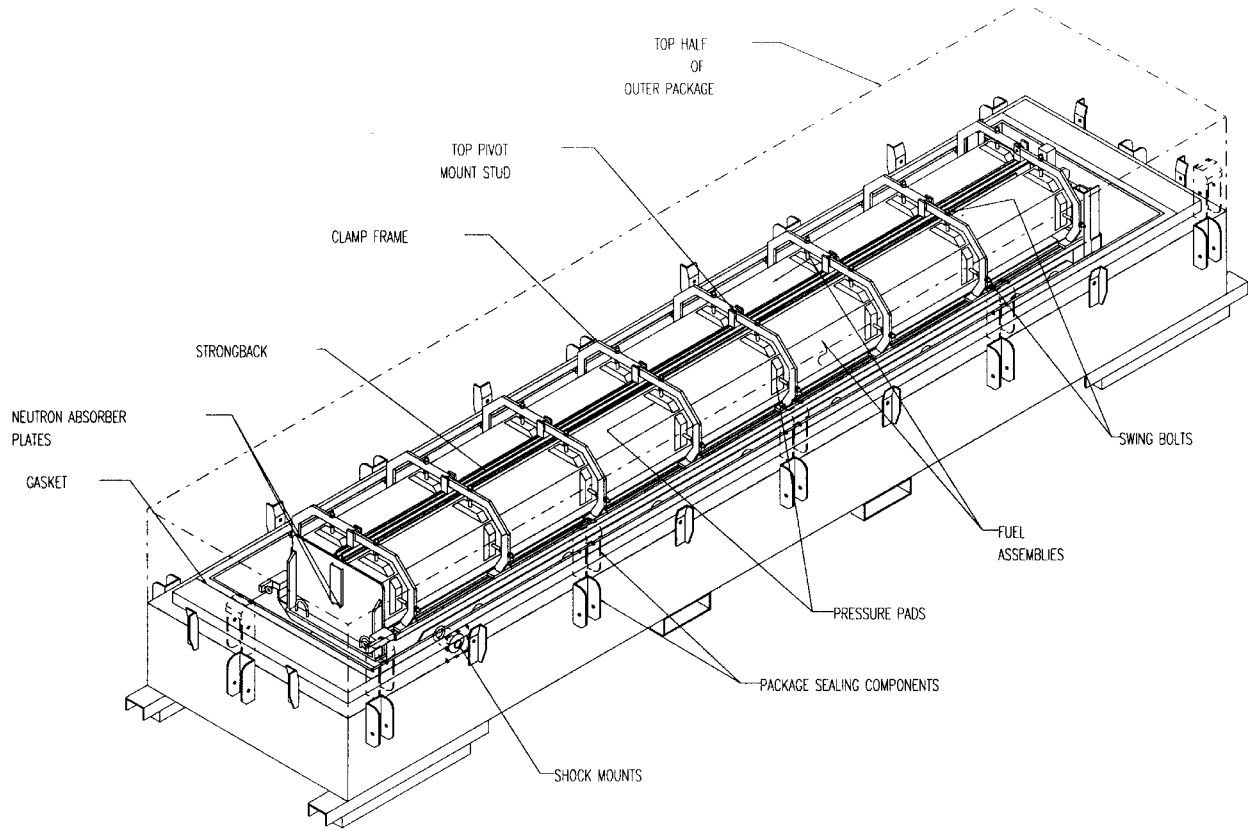


Figure 1. Isometric view of MO-1 transportation package.

### III. Establishment of Acceptance Criteria

A calculated  $k_{eff}$  for a fissile system is considered to be acceptably subcritical provided the calculated  $k_{eff}$  plus 2 standard deviations is less than a specified upper subcritical limit ( $USL$ ). The following relationship can be used to establish the acceptance criterion for a calculated multiplication factor for a subcritical system,  $k_s$  [5]:

$$k_s + 2\sigma \leq 1.00 + \beta - \Delta\beta - \Delta k_m, \quad (1)$$

where  $\beta$  and  $\Delta\beta$  represent the calculational bias and uncertainty in the calculational bias, respectively. The quantity  $\Delta k_m$  represents an administrative margin, and for transportation package applications, the minimum administrative margin of subcriticality is 5% (i.e.,  $\Delta k_m = 0.05$ ). The bias,  $\beta$ , in the calculational method is the difference between the mean value of the calculated  $k_{eff}$  for the critical experiments,  $k_c$ , and 1.0 (i.e.,  $\beta = k_c - 1$ ).

A *USL* is an upper subcritical limit such that there is a specified level of confidence that a calculated  $k_{eff}$  is considered to be subcritical. Using the acceptance criteria for a subcritical system with an administrative margin of 0.05, the *USL* can be defined as follows:

$$k_s + 2\sigma \leq USL = 0.95 + \beta - \Delta\beta. \quad (2)$$

A fissile system is considered to be acceptably subcritical provided the calculated  $k_{eff}$  plus 2 standard deviations is below the *USL*.

The calculational bias in the acceptance criteria can be positive if  $k_c$  is greater than one; however, a positive bias is not used in this study. Therefore, the bias is always less than or equal to zero. Regarding the uncertainty in the validation, the sources of uncertainty include the calculational method, the experimental data or technique and calculational models as well as the particular analyst. The sources of uncertainty are cumulatively observed in the variability of the calculated  $k_{eff}$  results obtained for the modeled critical experiments. Furthermore, this variability includes the Monte Carlo standard deviation in each calculated  $k_{eff}$  for the critical experiment as well as changes in the calculated value due to consideration of the experimental uncertainties. Consequently, the noted uncertainties are included in the bias and uncertainty in the bias.

#### IV. Traditional Validation Analysis

A criticality safety scoping study has been performed for the MO-1 package with WG MOX fuel in order to clarify and establish the criticality safety information that should be included in the safety application for the package [4]. In support of the initial criticality safety study and prior to the development of the S/U and GLLSM methods, traditional validation methods were used to validate the SCALE CSAS25 sequence [6] with the 238-group ENDF/B-5 cross-section library. The traditional approach involved the selection of 102 critical benchmark experiments that were **judged** to be similar to the MO-1 package with WG MOX fuel. The experiments consist of Pu systems as well as Pu-U mixtures in various chemical forms. The following discussion provides a summary of the validation study which is described in more detail in Ref. [4].

As noted previously, Eq. (2) represents the acceptance criterion for establishing subcriticality of a fissile system. In order to determine the *USL* for the application of interest, an estimate of the bias and uncertainty in the bias must be determined based on the evaluation of the set of 102 benchmark experiments. Moreover, the USLSTATS [7] code was used to calculate an upper subcritical limit (*USL*) as a function of each independent parameter using two different approaches: (1) a confidence band with administrative margin approach, and (2) a single-sided uniform-width closed-interval approach [i.e., lower tolerance band (LTB) method].

The *USL* obtained with the first method is defined with the following expression:

$$USL_1(x) = 1.0 - \Delta k_m - W + \beta(x). \quad (3)$$

$W$  is the confidence band width for the lower confidence limit.  $W$  is determined statistically based on a specified confidence level  $(1-\gamma_1)$  and the calculated  $k_{eff}$  values for the critical experiments. The lower confidence limit, which is  $k_c(x) - W$ , provides a  $(1-\gamma_1)$  confidence that the calculated  $k_{eff}$  values for the critical experiments are above the lower confidence limit. The confidence band is directly proportional to the standard deviation in the data and the specified level of confidence. A higher confidence level or larger standard deviation will lead to a larger value for  $W$ . The confidence band accounts for uncertainties in the experiments, the calculational method and data. Furthermore,  $W$  provides a statistical estimate for the uncertainty in the bias,  $\Delta\beta$ . USLSTATS provides an estimate for  $W$ . For the *USL* determination in the MO-1 validation, the confidence level is 95%.

In the LTB method, statistical techniques are used to determine a combined lower tolerance band plus subcritical margin. Moreover, the LTB approach yields a statistical estimate of  $\Delta k_m$  which is generally less than 0.05. The LTB method can be used to estimate the administrative margin and demonstrate the 0.05 administrative margin is acceptable for the given set of critical experiments. The *USL* as defined in the LTB approach is expressed as follows:

$$USL_2(x) = 1.0 - (C_{\alpha/\rho} * s_\rho) + \beta(x). \quad (4)$$

In the above expression,  $s_\rho$  is the pooled variance for the linear fit to the data,  $k_c(x)$ .  $C_{\alpha/\rho}$  is a statistically determined multiplier that is tabulated in most statistical handbooks for a specified confidence,  $\alpha$ , and probability,  $\rho$ . The term  $C_{\alpha/\rho} * s_\rho$  provides a lower tolerance band such that there is  $\alpha$  confidence that a future calculation of a critical system within the range of applicability will lie above the lower tolerance band with probability,  $\rho$ . The term  $C_{\alpha/\rho} * s_\rho$  can also be used to provide a statistical estimate of the administrative subcritical margin,  $\Delta k_m$ . Moreover,  $\Delta k_m$  is the difference between  $C_{\alpha/\rho} * s_\rho$  and the confidence band,  $W$  (i.e.,  $\Delta k_m = C_{\alpha/\rho} * s_\rho - W$ ).

Prior to establishing the *USL* for the MO-1 application, a series of calculational studies were performed to investigate possible trends in the set of 102 benchmark experiments. In addition, twelve different subsets of the benchmark suite were also investigated for possible trends that may be obscured by the entire set of criticals. The following steps were used to investigate the complete and partial set of benchmark experiments:

1. Identify independent parameters or variables for evaluation. The investigated variables include: H/<sup>239</sup>Pu, <sup>241</sup>Pu/<sup>239</sup>Pu, <sup>240</sup>Pu/<sup>239</sup>Pu, temperature, pitch, energy of average lethargy causing fission (EALF), atomic number density of Ga, B, Gd, Fe, N, O, H, <sup>239</sup>Pu, <sup>240</sup>Pu, <sup>241</sup>Pu, <sup>242</sup>Pu, <sup>235</sup>U and <sup>238</sup>U.
2. Calculate Pearson's product moment coefficient or correlation coefficient for the calculated  $k_{eff}$  values as a function of each independent variable for  $n$  experiments:

$$r_{x,y} = \frac{\sum xy - \frac{1}{n} \sum x \sum y}{(n-1)s_x s_y}, \quad (5)$$

where  $x$  is the independent parameter and  $y$  is the calculated  $k_{eff}$ . The sample standard deviation for  $x$  and  $y$  are denoted by  $s_x$  and  $s_y$ , respectively. The value of the correlation coefficient can range between  $-1$  and  $1$  indicating an inverse or direct correlation, respectively. A correlation coefficient equal to zero indicates no correlation between the calculated  $k_{eff}$  values and the corresponding independent variable. A correlation coefficient that lies between  $\pm 0.3$  is considered to be a weak correlation. Note that the Pearson correlation coefficient only provides an estimate of the correlation between the calculated  $k_{eff}$  values and the associated independent variable. As a result, the  $r_{x,y}$  values do not provide a direct correlation estimate between the benchmark experiments and the MO-1 application.

3. Calculate the significance level for the correlation coefficient that is calculated with Eq. (5). In order to estimate the significance of the correlation, a test statistic,  $t$ , is used to test the null hypothesis that the population correlation equals zero. The value of  $t$  for each  $x$   $y$  correlation can be calculated using the relation:

$$t = r_{x,y} (n - 2)^{1/2} (1 - r_{x,y}^2)^{-1/2}. \quad (6)$$

The probability or level of significance for accepting the null hypothesis (i.e., population correlation is zero) is obtained from a  $t$ -distribution for the calculated value of  $t$ . Consequently, the lower the significance level, the higher the degree of confidence that the computed correlation represents a true phenomena.

4. Identify the variables that exhibit a statistically significant correlation (i.e.,  $|r_{x,y}| \geq 0.3$ ) with respect to system multiplication. The subsequent steps are performed for the variables that are considered to have statistically significant correlation with respect to  $k_{eff}$ .
5. Perform Chi-square test to determine if calculated  $k_{eff}$  values are normally distributed as a function of each independent variable. Note that USLSTATS performs a Chi-square test for the calculated  $k_{eff}$ 's as a function of the selected independent variable.
6. Use USLSTATS to calculate  $USL_1(x)$  and  $USL_2(x)$  using Eqs. (3) and (4), respectively.

Initially, the above procedures were used to investigate the set of 102 critical benchmark experiments. Based on the trending analysis of the entire set of benchmarks, five independent variables, which are presented in Table 1, were determined to be acceptable parameters for establishing the  $USL$  for the MO-1 evaluation. The calculated  $USL$ s obtained with Eqs. (3) and (4) are presented for each independent variable in Table 1 along with the associated range of applicability.

Although the  $USL$  has functional dependence with respect to each independent parameter, the subcritical limits that are presented in Table 1 represent the minimum value of the  $USL$  in the range of applicability. For each independent variable, the  $\Delta k$  bias,  $\beta$ , is provided with the estimated uncertainty. If a positive bias is obtained, the bias is set equal to zero for the  $USL$  determination.

Based on the LTB method, an estimate of the administrative margin is obtained and presented in Table 1. For each independent variable, the subcritical limit obtained with the 5% administrative margin leads to a much lower and conservative *USL* relative to the LTB approach.

The calculated *USLs* obtained for the H atom density and H/<sup>239</sup>Pu are slightly lower relative to the three remaining variables in Table 1. Because the ratio of H to <sup>239</sup>Pu provides information about the amount of fissile material in the system and the degree of hydrogen moderation, H/<sup>239</sup>Pu was selected as the independent variable for the criticality safety study of the MO-1 package. The calculated *USLs* for  $k_{eff}$  as a function of H/<sup>239</sup>Pu and H atom density are essentially equivalent except in the low moderation range. In particular, there is a negative bias for H atom densities below 0.033. In an effort to account for the negative bias associated with the lower H atom densities, the *USL* of 0.9354 for H/<sup>239</sup>Pu was reduced to 0.9285.

Table 1. Summary of *USL* Calculations for 102 Critical Experiments

Variable	$\beta$ (%)	$\Delta\beta$ (%)	$USL_1$ ( $\Delta k_m = 5\%$ )	LTB Method		
				$USL_2$	Est. $\Delta k_m$ (%)	Range of App. <sup>a</sup>
H/ <sup>239</sup> Pu	0.24	1.46	0.9354	0.9690	1.65	$0 \leq x \leq 2437$
H	-0.73	1.42	0.9285	0.9627	1.57	$0 \leq x \leq 0.0667$
N	0.31	1.41	0.9359	0.9696	1.63	$0 \leq x \leq 0.0443$
<sup>241</sup> Pu/ <sup>239</sup> Pu	0.36	1.39	0.9361	0.9711	1.5	$0 \leq x \leq 0.26$
<sup>240</sup> Pu/ <sup>239</sup> Pu	0.30	1.41	0.9359	0.9706	1.53	$0.0178 \leq x \leq 1.0342$

<sup>a</sup> For nuclide or isotopic variables the units are atoms/barn-cm.

Note that the acceptance criteria that is presented in Table 1 is based on the evaluation of the complete set of benchmark experiments. It is prudent to examine subsets of the suite of benchmarks to ensure that possible trends in the calculated  $k_{eff}$  values as a function of the independent parameters are not obscured by the entire set of criticals. As noted previously, trending analyses and *USL* calculations (i.e., Steps 1 through 6) were repeated for 12 different subsets of the experimental database, and the different subsets of the benchmark database are provided in Table 2.

As noted in Table 1, the range of H/<sup>239</sup>Pu values for the 102 experiments extends between 0 and 2437; however, the range of H/<sup>239</sup>Pu values for the MO-1 evaluation only extends between 0 and 111. In the experimental database, 36 of the experiments have H/<sup>239</sup>Pu ratios below 126.4, and this subset is identified in Table 2. Because of the large range of moderation ratios in the complete set of experiments, the smaller 36-experiment subset was investigated for possible trends in the data. As with the complete set of experiments, each independent variable was investigated for the 36-experiment subset. Based on the evaluation of the different independent variables, the H/<sup>239</sup>Pu ratio yields the most conservative *USL*; however, the evaluation of the subset revealed a negative bias ( $\beta = -0.3\%$ ) for H/<sup>239</sup>Pu values between 0 and 51.1 that was obscured by the larger set of criticals.



Although there is a negative bias associated with the 36-experiment subset, the uncertainty in the bias is 0.98% which is ~1.5 times smaller relative to the complete set of benchmarks. As a result, the calculated *USL* for the 36-experiment subset is 0.9373 which is less conservative relative to the *USL* obtained for the complete set of experiments.

Table 2. Experimental Subsets for Validation Analysis

Subset Description	Number of experiments
Experiments with H/ <sup>239</sup> Pu ratios below 126.4	36
Mixed Pu-U experiments	32
Pu experiments	70
H <sub>2</sub> O moderated experiments	83
H moderated experiments	101
Experiments with neutron absorbers	28
H <sub>2</sub> O reflected experiments	61
Experiments involving carbon	30
Experiments involving nitrogen	73
Experiments involving structural steel	63
Experiments involving cylindrical or annular geometry	68
Array experiments	28

The trending analyses and *USL* calculations that are documented in Steps 1 through 6 were also performed for the remaining subsets of experiments in Table 2. For each subset of experiments, *USL*s were calculated for each independent variable exhibiting a statistically significant correlation with  $k_{eff}$ . Based on the study of the partial sets of experiments, an independent variable with a stronger correlation to  $k_{eff}$  may lead to a less conservative *USL* relative to an independent variable with a weaker correlation to system multiplication. A summary of the evaluation of the experiment subsets is provided in Table 3. The variables that are presented in Table 3 have a minimum  $USL_1(x)$  value that is less than the *USL* for H/<sup>239</sup>Pu (0.9354).

As noted in Table 3, there is a statistically significant correlation between  $k_{eff}$  and EALF for the water-moderated and water-reflected experiments. The majority of experiments have EALF values below 0.3 eV which indicates the systems are well moderated. For the water-moderated and water-reflected experiment subsets, the minimum *USL* is lower relative to the *USL* as a function of hydrogen moderation for the entire set of experiments. Therefore, for the MO-1 evaluation, the *USL* was lowered to **0.9245** to account for negative biases as a function of EALF for the water-moderated and reflected experiments.

Table 3. *USL* Calculations for Selected Experiment Subsets

Variable	$\beta$ (%)	$\Delta\beta$ (%)	LTB Method		Est. $\Delta k_m$ (%)	Range of App. <sup>a</sup>
			$USL_1$ ( $\Delta k_m = 5\%$ )	$USL_2$		
<u>H<sub>2</sub>O Moderated Experiments</u>						
H/ <sup>239</sup> Pu	0.40	1.47	0.9353	0.9683	1.7	$11.189 \leq x \leq 2437.3$
EALF	-0.88	1.67	0.9245	0.9544	2.01	$0.019 \leq x \leq 1.017$
<sup>239</sup> Pu	-0.50	1.46	0.9304	0.9634	1.7	$3 \times 10^{-5} \leq x \leq 4.2 \times 10^{-3}$
<u>H Moderated Experiments</u>						
H	-0.31	1.37	0.9332	0.9698	1.43	$0.0242 \leq x \leq 0.0667$
<sup>239</sup> Pu	-0.26	1.43	0.9331	0.9676	1.55	$3 \times 10^{-5} \leq x \leq 4.2 \times 10^{-3}$
<u>H<sub>2</sub>O Reflected Experiments</u>						
EALF	-0.75	1.71	0.9254	0.9538	2.15	$0.019 \leq x \leq 1.017$
<sup>239</sup> Pu	-0.62	1.36	0.9302	0.9637	1.65	$3 \times 10^{-5} \leq x \leq 4.2 \times 10^{-3}$
<sup>240</sup> Pu	-0.18	1.46	0.9336	0.9659	1.77	$1.5 \times 10^{-6} \leq x \leq 5.6 \times 10^{-4}$
<sup>235</sup> U	-0.10	1.38	0.9352	0.9689	1.63	$0 \leq x \leq 3 \times 10^{-4}$
<sup>238</sup> U	-0.09	1.38	0.9353	0.9690	1.63	$0 \leq x \leq 0.0412$
<u>Experiments with Structural Steel</u>						
<sup>239</sup> Pu	-0.48	1.4	0.9312	0.9643	1.69	$3 \times 10^{-5} \leq x \leq 4.2 \times 10^{-3}$
<u>36 Experiment Subset ( <math>0. \leq H^{239}\text{Pu} \leq 126.42</math> )</u>						
<sup>238</sup> U	-0.58	1.02	0.9340	0.9707	1.33	$0 \leq x \leq 0.0169$

<sup>a</sup> For nuclide or isotopic variables the units are atoms/barn-cm.

## V. S/U and GLLSM Analysis Methods

In the previous sections, a "traditional" approach is presented for validating the CSAS25 sequence of the SCALE code system using the 238-group ENDF/B-5 cross-section library. As part of the validation, a calculational *USL* is established for evaluating the shipment of WG MOX fuel in the MO-1. The experiments were selected based on engineering judgment and perceived applicability to the MO-1 transportation package. Because of the judgment associated with the traditional approach, the applicability or similarity of the benchmark experiments to the application of interest is somewhat subjective.

As noted previously, the S/U and GLLSM methods development occurred subsequent to the initial validation study for the MO-1 application. In order to gain experience with the S/U and GLLSM

methodology, the validation for the MO-1 package was revisited using the S/U and GLLSM analysis procedures. Moreover, the objective of the analysis is to determine whether the benchmark experiments are applicable to the MO-1 package. In addition, the purpose of the work is to estimate the bias and uncertainty in the bias for the MO-1 evaluation. Based on the bias and associated uncertainty, a new *USL* can be calculated and compared with the traditional validation approach.

The S/U methods have been used to assess the applicability of the benchmarks to the MO-1 package. The similarity of the benchmarks to the MO-1 package has been determined by using S/U analysis techniques that involve the determination of sensitivity coefficients for the MO-1 application models and the set of critical benchmarks. Based on the procedures of Ref. [3], parameters that are denoted as *E* values have been calculated for the MO-1 relative to the set of benchmarks. The *E* values are defined as follows [3]:

$$E_f = M^{-1} \sum_{j=1}^N \sum_{i=1}^g S_{faij} S_{feij} , \quad (7)$$

$$E_s = M^{-1} \sum_{j=1}^N \sum_{i=1}^g S_{saij} S_{seij} , \quad (8)$$

$$E_c = M^{-1} \sum_{j=1}^N \sum_{i=1}^g S_{cai} S_{ceij} , \quad (9)$$

and

$$M = \sum_x \left[ \sum_{j=1}^N \sum_{i=1}^g (S_{xaij})^2 \sum_{j=1}^N \sum_{i=1}^g (S_{xeij})^2 \right]^{1/2} , \quad (10)$$

where *S* is the sensitivity of  $k_{eff}$  for either the experimental configuration *e* or the application of interest *a* to the fission, scatter or capture cross sections (*f*, *s* or *c*, respectively) for energy group *i* and isotope/nuclide *j*. A cumulative sensitivity parameter *E* can also be defined as follows:

$$E = E_f + E_s + E_c . \quad (11)$$

The *E* coefficients represent the summation of the product of the sensitivity coefficients for two systems over all energy groups and nuclides. Moreover, the *E* coefficients are normalized such that an *E* value of 1 indicates that the two systems are equivalent, and an *E* value of 0 indicates the two systems are completely dissimilar. The *E* coefficients can be used to establish similarity or lack thereof between two systems based on the magnitude and shape of the sensitivity profiles for fission, scatter and capture. Systems that have an *E* coefficient between 0.8 and 1.0 are considered to be similar for validation purposes [3, 8].

In addition to sensitivity parameters, cross-section uncertainty information can be used to investigate system similarity. Uncertainty analysis techniques involve the propagation of cross-section uncertainty information to the calculated multiplication factor for a system [9]. Essentially, the determination of uncertainty in the system multiplication to the underlying nuclear data is a two-step

process. Typically, cross-section evaluators provide uncertainty information for a particular isotope/nuclide. The processing code PUFF [10] is used to process the nuclear data uncertainties from an ENDF (Evaluated Nuclear Data File) evaluation into a multigroup form for each isotope/nuclide. Once the nuclear data uncertainties are established, the uncertainty in the system multiplication to the data uncertainties is obtained by folding the cross-section uncertainties with the calculated sensitivity parameters that describe the changes in  $k_{eff}$  due to changes in each reaction for a material [9]:

$$C_{kk} = S_k C_{\alpha\alpha} S_k^T, \quad (12)$$

where  $T$  indicates the transpose of the sensitivity matrix  $S_k$ , and  $C_{\alpha\alpha}$  is the cross-section uncertainty matrix.

In Eq. (12),  $S_k$  is an  $I \times N$  matrix, where  $I$  is the number of systems being considered and  $N$  is the number of nuclear data parameters in the problem (e.g., number of isotope/nuclide reaction processes times the number of energy groups). Moreover,  $C_{\alpha\alpha}$  is an  $N \times N$  matrix that provides the cross-section uncertainty data for each reaction process in an energy group. The resulting  $C_{kk}$  matrix is an  $I \times I$  matrix that provides the covariance (i.e., shared or common variance),  $\sigma_{ij}^2$ , between systems  $i$  and  $j$  due to the underlying cross-section data uncertainties. In addition, the diagonal elements of the  $C_{kk}$  matrix represent the variance,  $\sigma_i^2$ , for each system due to the nuclear data uncertainties.

For convenience, each covariance element  $\sigma_{ij}^2$  of the  $C_{kk}$  matrix can be divided by the respective standard deviation for systems  $i$  and  $j$  to yield a correlation coefficient matrix. Each correlation coefficient is defined as  $c_k = \sigma_{ij}^2 / \sigma_i \sigma_j$ , and each coefficient represents the correlation between nuclear data uncertainties in systems  $i$  and  $j$ . Because cross-section data uncertainties for a particular isotope/nuclide are propagated to a system consisting of the material, two systems with the same material and similar spectra will be correlated. Likewise, systems with different materials or spectra will be uncorrelated. A  $c_k$  value of +1 represents a full correlation between systems  $i$  and  $j$ , and a correlation coefficient of -1 represents a complete anticorrelation between the two systems. In addition, a zero-valued correlation coefficient represents no correlation between systems  $i$  and  $j$ . Two systems with a  $c_k$  value  $> 0.8$  are considered to be similar for validation purposes [9].

In addition to the two S/U methods developed at ORNL to compare fissionable systems based on sensitivity and uncertainty information ( $E$  and  $c_k$ ). A Generalized Linear Least-Squares Methodology (GLLSM) procedure has also been developed to establish computational/nuclear data biases [8, 11]. The GLLSM procedure is an alternative approach to the traditional trending analysis for the determination of biases. Although the GLLSM procedure is classified with the S/U methods in this paper, the methodology is different from the S/U methods. Physically, the GLLSM is designed to "force agreement" between the measured and calculated values of  $k_{eff}$  by predicting data changes based on the entire set of critical experiments used in the data validation process. The data needed for such an analysis are almost identical to those in the S/U methods presented thus far: the sensitivity coefficients, the cross-section uncertainties, and the calculated and measured  $k_{eff}$  values with the addition of an estimate of the uncertainty in the measured  $k_{eff}$  values. The "data changes" that result

from the application of the GLLSM can then be used to predict (via interpolation or extrapolation) the biases for any application determined to be similar to the suite of benchmark experiments. A detailed description of the GLLSM procedure is provided in Ref. [11].

## VI. S/U and GLLSM Analyses for MOX Package

Two objectives for the S/U and GLLSM analyses are to quantitatively determine if the suite of benchmarks are applicable to the MO-1 package evaluation, and if the suite of benchmarks are applicable, estimate the  $\Delta k$  bias and uncertainty relative to the traditional validation approach.

In order to accomplish the two objectives, energy dependent sensitivity coefficients, or profiles, have been calculated for each nuclide reaction for each experiment in the benchmark suite using the 238-group ENDF/B-5 library with the SEN3 [12] sequence that has been developed at ORNL. In addition, sensitivity profiles were also calculated for the most reactive undamaged and damaged package models of the MO-1 with WG MOX fuel. The undamaged package model contains one WG MOX assembly and is optimally moderated and fully reflected with water. The damaged MO-1 package model, which also has one MOX assembly, has crushed exterior walls and is optimally moderated. Additional details of the package models and calculations are provided in Ref. [4].

Once the sensitivity profiles for the suite of benchmarks and MO-1 application were calculated with SEN3, the CANDE [13] code was used to calculate the  $c_k$  and  $E$  parameters between each benchmark experiment and each MO-1 package configuration. In an effort to demonstrate the results,  $k_{eff}$  values as a function of the  $c_k$  coefficients for the undamaged MO-1 package are provided in Figure 2. Based on the uncertainty analysis, 86 experiments have  $c_k$  values  $> 0.8$  relative to the undamaged MO-1 package. The  $c_k$  coefficients represent the sensitivity of  $k_{eff}$  to the individual cross-sections weighted by the cross-section uncertainties [9]. Therefore, experiments with the same materials and similar spectra should be characterized by significant correlation ( $> 0.8$ ) coefficients indicating a strong correlation between the experiments and the application. Based on the uncertainty analysis, the relatively large number of experiments with significant correlations indicate that the suite of benchmarks are similar to the undamaged MO-1 package. Thus, the uncertainty analysis demonstrates that the suite of benchmark experiments are applicable to the undamaged MO-1 package evaluation.

Using the procedures from Ref. [8], a trending analysis can be performed with the  $c_k$  values for the benchmarks relative to the application of interest. The linear regression for  $k_{eff}$  as a function of the correlation coefficient is also provided in Figure 2. Note that a  $c_k$  value of unity represents a full correlation with the application of interest. As a result, the estimated bias in system multiplication is obtained by extrapolating the linear fit for  $k_{eff}$  to a  $c_k$  value of unity. Based on the extrapolation, the  $\Delta k$  bias is 0.57%. The uncertainty in the bias is estimated by calculating the standard error of prediction associated with the extrapolation and multiplying by the appropriate t-statistic for a specified confidence level and degrees of freedom. For a 95% confidence level, the estimated uncertainty in the bias is 1.6%.

Note that the uncertainty in the bias is obtained by estimating the standard error of the predicted  $k_{eff}$  at a  $c_k$  value of 1. As the mean  $c_k$  value for the suite of benchmarks approaches unity, the standard error of prediction decreases because the extrapolation range becomes smaller. For the trending analysis in Figure 2, 65 experiments have a  $c_k$  value  $> 0.9$ , and 20 experiments have a  $c_k$  value  $> 0.95$ .

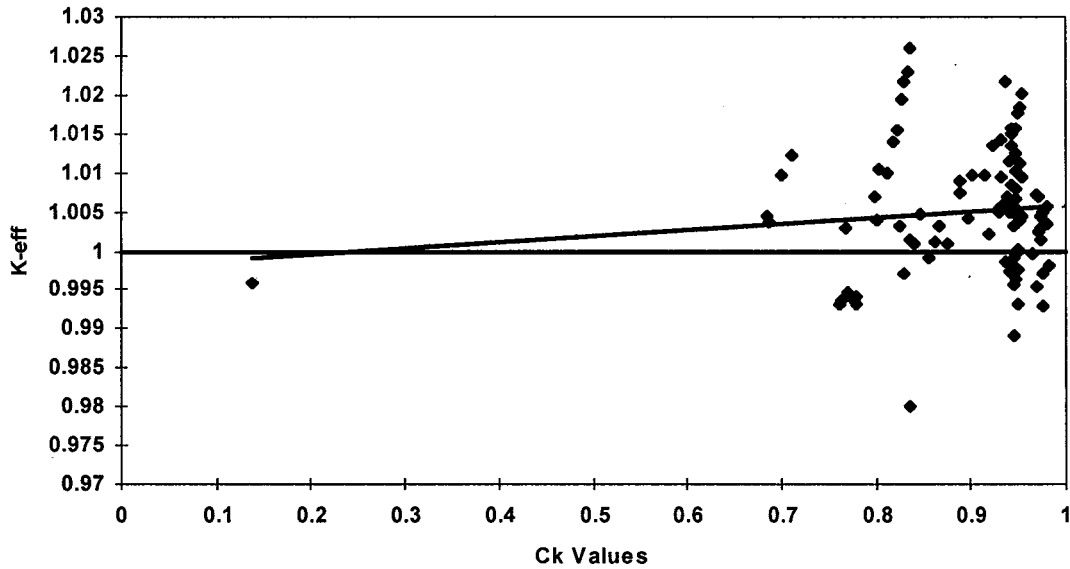


Figure 2. Trend Plot of  $k_{eff}$  with  $c_k$  Values for Undamaged MO-1 Package.

For the damaged packaged, 76 experiments have  $c_k$  values  $> 0.8$  which also indicates that the suite of benchmarks are applicable to the damaged package analysis. Based on a trending analysis for  $k_{eff}$  as a function of the correlation coefficient, the  $\Delta k$  bias and associated uncertainty are 0.58% and 1.61%, respectively.

Similar trending procedures can be used to estimate the calculational bias and uncertainty based on the calculated  $E$  coefficients. Estimates of the  $\Delta k$  bias and uncertainty are provided in Table 4 for trending analyses as a function of the  $c_k$  and  $E$  parameters for each MO-1 package configuration. Note that results from the trending analyses are also presented in Table 4 for experiments with  $c_k$  and  $E$  values that are  $> 0.8$ . By examining the smaller sets of experiments, different estimates of the bias and uncertainty are obtained. As indicated in Table 4, trending as a function of  $E$  for the damaged package leads to a bias of  $-0.53\%$  with an uncertainty of 2.11%. The large uncertainty in the bias is attributed to the small set of experiments (i.e., 28 experiments) relative to the entire suite with  $E$  values that range between 0.8 and 0.87. Because the range of  $E$  values for the damaged package are in the 0.8 range, the extrapolation region is much larger relative to the other experiment subsets. As a result, the standard error of prediction at an  $E$  value of 1 increases as the extrapolation region becomes larger.

Table 4. Comparison of Predicted  $\Delta k$  Bias and Uncertainty for S/U and GLLSM Procedures

Procedure	Undamaged MO-1		Damaged MO-1	
	Bias (%)	Bias Uncertainty (%)	Bias (%)	Bias Uncertainty (%)
$c_k$ (All Exps)	0.57	1.6	0.58	1.61
$E$ (All Exps)	0.71	1.5	0.59	1.63
$c_k > 0.8$	0.32	1.58	-0.14	1.42
$E > 0.8$	-0.31	1.6	-0.53	2.11
GLLSM (All Exps)	0.20	0.24	-0.09	0.45
GLLSM ( $c_k > 0.8$ )	0.11	0.26	-0.89	0.58
GLLSM ( $E > 0.8$ )	0.16	0.28	-0.58	1.01

Estimates of the  $\Delta k$  bias and uncertainty based on the GLLSM procedure are also provided in Table 4. In the GLLSM approach, a data adjustment procedure is used to determine the "best" cross sections that are needed to calculate the  $k_{eff}$  for the suite of benchmark experiments. Based on the procedures of Ref. [8], an estimate of the  $\Delta k$  bias is obtained by multiplying the sensitivity for the application (i.e., sensitivity of calculated  $k_{eff}$  for the application to the cross-section data) by the changes in the cross-section data that are obtained from the data adjustment procedure for the suite of benchmark experiments. The uncertainty in the bias obtained with the GLLSM procedure is estimated by calculating the standard error of prediction multiplied by the appropriate t-statistic for a 95% confidence level and specified degrees of freedom. The standard error of prediction in the GLLSM approach includes the standard deviation in the adjusted  $k_{eff}$  for the application (i.e., system multiplication that would be obtained using the adjusted or "best" cross sections). As noted in Ref. [11], caution is advised with the use of the bias uncertainty from GLLSM because the development of the statistical basis is currently under development.

In Table 4, GLLSM results are also presented for the subsets of experiments that are characterized with  $c_k$  and  $E$  values above 0.8. Different biases are obtained by performing the GLLSM procedure for the different experiment subsets. Because nuclear data adjustments are performed in the GLLSM procedure, the data adjustments are dependent on the number of experiments considered. When the GLLSM is applied to the entire suite of experiments, the data adjustments are determined based on the entire suite of experiments. Therefore, the data changes for an experiment that is considered to be similar to the application of interest must also be tempered against an experiment that may not be similar to the application. When the GLLSM is applied to the smaller set of experiments, the data changes are only applicable for the smaller experimental subset without consideration of the other experiments in the suite of benchmarks.

The S/U and GLLSM results in Table 4 demonstrate that different estimates of the bias and associated uncertainty can be obtained by trending with the complete suite of experiments relative to the suite of experiments that are determined to be similar to the application of interest. In some cases, different estimates of the bias can be obtained by trending as a function of  $c_k$  relative to  $E$ . Moreover, different bias estimates can be obtained with the GLLSM procedure relative to the S/U methods. As indicated previously, the objective of this paper is to gain experience with the application of the S/U and GLLSM procedures to a Pu-U system. However, guidance for the use of these procedures for Pu-U systems is not completely finalized, and work is currently in progress to develop guidance for the use of the S/U and GLLSM procedures for Pu-U systems.

Despite the limited availability of guidance for Pu-U systems, the S/U and GLLSM procedures can be used to identify experiments that are similar to the MO-1. In addition, the S/U and GLLSM procedures can be used to establish bounding values for the  $\Delta k$  bias and associated uncertainty that can be compared with the traditional validation results for the MO-1.

Based on the results in Table 4, the lowest  $USL$  value is obtained from the trending analysis of  $k_{eff}$  as a function of  $E$  values that are greater than 0.8 relative to the damaged MO-1 configuration. Using a 5% administrative margin with a -0.53% bias and 2.11% bias uncertainty, a value of **0.9236** is obtained for the  $USL$  based on the S/U procedures. As noted previously, the  $USL$  obtained with the traditional validation procedure is **0.9245** which is slightly higher but consistent with the S/U analyses. In the traditional validation, the 0.9245  $USL$  was determined from trending analyses of  $k_{eff}$  as a function of EALF for the H<sub>2</sub>O-moderated subset of experiments. In the S/U analysis, 28 experiments have  $E$  values  $> 0.8$  relative to the damaged MO-1 configuration, and 24 of the 28 cases are the same H<sub>2</sub>O-moderated experiments that were examined as a function of EALF in the traditional validation. The remaining 4 experiments also have H moderation. These results demonstrate the capability of the S/U methods to identify the experiments that are important for validation purposes.

Using the S/U and GLLSM methods, the similarity of each benchmark experiment relative to the MO-1 package models has been determined quantitatively. In addition, the S/U and GLLSM procedures have been used to estimate the  $\Delta k$  bias and uncertainty in the bias for the most reactive damaged and undamaged MO-1 package configurations with WG MOX fuel. The results obtained with the S/U and GLLSM methods support the traditional validation analysis for the MO-1 package with WG MOX fuel. These results demonstrate the capability of the S/U and GLLSM procedures for performing validation studies and/or assessing traditional validation analyses.

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