

**Log Number: 2.3BB28**  
**Topic Area Number: 2.3**  
**Oral Presentation**

Computational Physics and Engineering Division

## **Proposed Methodology for Establishing Area of Applicability**

**B. L. Broadhead, C. M. Hopper, and C. V. Parks**

Oak Ridge National Laboratory,\*

P. O. Box 2008,

Oak Ridge, TN 37831-6370

e-mail: bub@ornl.gov

phone: (423) 576-4476

fax: (423) 576-3513

e-mail: fhh@ornl.gov

phone: (423) 576-8617

fax: (423) 576-3513

e-mail: cvp@ornl.gov

phone: (423) 574-5280

fax: (423) 576-3513

Submitted to the

ICNC'99

Sixth International Conference on Nuclear Criticality Safety,

September 20–24, 1999,

Palais des congrès . Versailles . France

The submitted manuscript has been authored by a contractor of the U.S. Government under contract No. DE-AC05-96OR22464. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

---

\*Managed by Lockheed Martin Energy Research Corporation under contract DE-AC05-96OR22464 for the U.S. Department of Energy.

## PROPOSED METHODOLOGY FOR ESTABLISHING AREA OF APPLICABILITY

**B. L. Broadhead, C. M. Hopper, and C. V. Parks**  
Oak Ridge National Laboratory, U.S.A.

### Abstract

This paper presents the application of sensitivity and uncertainty (S/U) analysis methodologies to the data validation tasks of a criticality safety computational study. The S/U methods presented are designed to provide a formal means of establishing the area (or range) of applicability for criticality safety data validation studies. The development of parameters that are analogous to the standard trending parameters form the key to the technique. These parameters are the so-called D parameters, which represent the differences by energy group of S/U-generated sensitivity profiles, and  $c_k$  parameters, which are the correlation coefficients, each of which give information relative to the similarity between pairs of selected systems. The use of a Generalized Linear Least-Squares Methodology (GLLSM) tool is also described in this paper.

These methods and guidelines are also applied to a sample validation for uranium systems with enrichments greater than 5 wt %.

### Introduction

The validation requirements concerning criticality safety in the U.S. are described in ANSI/ANS-8.1-1998, which defines the area(s) of applicability as follows: **“the limiting ranges of material compositions, geometric arrangements, neutron energy spectra, and other relevant parameters (such as heterogeneity, leakage, interaction, absorption, etc.) within which the bias of a calculational method is established.”**

The standard also notes that **“the area(s) of applicability of a calculational method may be extended beyond the range of experimental conditions over which the bias is established by making use of trends in the bias. Where the extension is large, the method should be supplemented by other calculational methods to provide a better estimate of the bias, and especially of its uncertainty in the extended area (or areas), and to demonstrate consistency of computed results.”**

The establishment of these areas of applicability are vague in that no guidance is given with respect to determining what constitutes a valid range, or under what conditions the range is breached. The second statement does little to clarify the situation in that the methods used to extend the areas of applicability are not stated.

A useful tool in establishing similarities between systems is the use of so-called sensitivity coefficients. Physically, sensitivity coefficients are defined such that they represent the percentage effect on some response due to a 1 percent change in an input parameter. For critical systems, an appropriate response is the system  $k_{\text{eff}}$  value, with the input parameters of interest being the nuclear reaction probabilities or cross sections. These sensitivities can be presented either as “total” sensitivities, where the cross-section change

is uniform over all energies, or as a “profile,” where the change in  $k_{\text{eff}}$  due to cross sections is given as a function of the energy of the cross section. In this application, the full-sensitivity profiles are generated in the selected problem neutron-energy-group structure for each material and reaction type (i.e.,  $^{235}\text{U}$  fission, scatter,  $\sigma_{\text{P}}$ , capture, etc.). In a criticality safety validation study, typically some 30–50 critical benchmarks are used. Sensitivity profiles give a great deal of information about the particular system; however, the amount of information is too large to be of general use (20 profiles for each system, with about 40 values each, i.e., one for each energy group). Therefore, a method of obtaining the differences between the sensitivity profiles for pairs of systems was devised to reduce the amount of needed information to only a few parameters, while maintaining the uniqueness of the information present in the full-sensitivity profiles. The most promising set of parameters are a family of so-called “D” values as defined below:

$$D_n = \sum_{i=1}^g \#_{\text{nai}} - S_{\text{nei}} \quad D_c = \sum_{i=1}^g \#_{\text{cai}} - S_{\text{cei}} \quad D_s = \sum_{i=1}^g \#_{\text{sai}} - S_{\text{sei}},$$

where  $S$  is the sensitivity of  $k_{\text{eff}}$  for the safety application, a, or experimental configuration, e, to the capture and scattering cross sections, or to  $\sigma_{\text{c}}$ ,  $\sigma_{\text{s}}$ , or  $\sigma_{\text{n}}$ , respectively) for group  $i$ . These coefficients are useful in making a quick determination of the similarity between pairs of systems.

An alternative approach to exploring the similarity of systems is to use uncertainty analyses. This procedure involves the propagation of estimated cross-section uncertainty information to the calculated  $k_{\text{eff}}$  value of a given system via the sensitivity coefficients. Mathematically this is accomplished by a quadratic product of the sensitivity profile vectors for each system, material, and reaction type with the cross-section uncertainty matrices by material and reaction type. The result of this procedure is not only an estimate of the uncertainty in the system  $k_{\text{eff}}$  for a given system, but also an estimate of the correlated uncertainty *between* systems. These correlated uncertainties can be represented by correlation coefficients, which effectively represent the degree of correlation (0 = no correlation, 1 = full correlation, -1 = full anticorrelation) in the uncertainties between the two systems. This parameter, denoted as  $c_k$ , has not only the desirability of a single quantity relating the two systems, but the similarity of the systems is measured in terms of uncertainty, not just sensitivity.

A final approach to the traditional trending analysis for determination of biases is the use of the so-called Generalized Linear Least-Squares Methodology (GLLSM). Physically the GLLSM is designed to “force agreement” between the measured and calculated values of  $k_{\text{eff}}$  for the entire set of criticals used in the data validation process. The inputs needed for such an analysis are almost identical to the concepts presented thus far; the sensitivity coefficients, the cross-section uncertainties, the actual calculated and measured  $k_{\text{eff}}$  values, with the addition of an estimate of the uncertainty in the measured  $k_{\text{eff}}$  values. Mathematically the GLLSM represents a combination of measurements. These measurements include the experimental values of  $k_{\text{eff}}$  for each critical benchmark and the calculated value of  $k_{\text{eff}}$  obtained via functional analysis of the cross-sections measurements. The “data changes” that result from the application of the GLLSM can then be used to predict the biases for *any* similar application where the area of application corresponds to an interpolation or extrapolation scenario.

This paper describes an illustrative application of both the S/U and GLLSM procedures to the validation of criticality safety studies for facilities processing commercial reactor fuels with uranium enrichments greater than 5 wt %. In the past, these processing facilities have been limited to enrichments at or below 5 wt %. Hence, much of the critical experiment data correspond to these lower enrichments. The use of S/U and GLLSM methods in validation studies was demonstrated by performing a validation of a hypothetical set of application scenarios, which consist of 14 systems each having  $\text{U}(11)\text{O}_2$  fuel with H/X values varying from 0 to 1000. The 11-wt % enrichment was chosen so that critical systems that exist over the entire range of moderations, including dry, could be studied. The data validation included both the traditional trending analyses, trending analysis with the  $D$  and  $c_k$  parameters, and finally the full GLLSM approach. Advantages and disadvantages of each approach were explored, and guidance for general use of these techniques was developed.

## Sensitivity Coefficient Methods

The techniques used in this work to generate sensitivity information for the various critical benchmarks is based on the widely used perturbation theory approach [1–4]. The full derivation of the general procedure will not be given here; however, for the specific theory and code development for the generation of  $k_{\text{eff}}$  sensitivities, the reader is referred to the accompanying paper [5].

The  $k_{\text{eff}}$  sensitivity, as described above, has been implemented by modifying a version of the FORSS [6] (Fantastic Oak Ridge Sensitivity System) package. The FORSS system was developed in the late 1970s, primarily for use in the development of fast reactor systems.

This project has reactivated the individual FORSS modules, with the goal of putting portions of the original system into the SCALE [7] system. A one-dimensional (1-D) sensitivity sequence, SEN1 [8], was produced for use in this project and for subsequent general use. The capacity to generate 2-D sensitivities is also available via the SEN2 module. More complete information on SEN1 and SEN2, the progress to date on 3-D Monte Carlo methods, and some results of using the SEN1 and SEN2 capabilities are the subject of a companion paper [5].

## Uncertainty Analysis Theory

The determination of uncertainties in the calculated values of the system multiplication factor is accomplished by two steps: the estimation/processing of uncertainties in the underlying cross-section data and the propagation of those uncertainties to the system  $k_{\text{eff}}$  value. The techniques for processing cross-section uncertainty data are well-known [9,10] and will not be discussed here.

Once cross-section uncertainty information for all materials and reaction processes that are important to the systems of concern are available, it is then possible to estimate the uncertainty in the system multiplication factor due to these data uncertainties. If we denote the matrices of uncertainty information for all of the cross sections as  $C_{\text{xxx}}$  and the sensitivity matrices relating changes in each constituent material and process to the system  $k_{\text{eff}}$  as  $S_k$ , the uncertainty matrix for the system  $k_{\text{eff}}$  values,  $C_{\text{kk}}$  is given as:

$$C_{\text{kk}} = S_k C_{\text{xxx}} S_k^T.$$

The  $S_k$  matrix is  $I \times N$ , where  $I$  is the number of critical systems being considered, and  $N$  is the number of nuclear data parameters in the problem. Typically  $N$  is the number of material/reaction processes times the number of energy groups. The  $C_{\text{xxx}}$  matrix is an  $N \times N$  matrix, with the resulting  $C_{\text{kk}}$  matrix  $I \times I$ . The  $C_{\text{kk}}$  matrix consists of variance values for each of the critical systems under consideration (the diagonal elements), as well as the so-called “covariance” between systems (the off-diagonal elements). These off-diagonal elements represent the shared or common variance, hence the term covariance, between the various systems. For presentation, these off-diagonal elements are typically divided by the square root of the corresponding diagonal elements (i.e., the respective standard deviations) to generate a correlation coefficient matrix.

These  $c_k$  values are felt to be most appropriate for correlation with error trends in a criticality safety validation analysis because they are essentially the sensitivities to the individual cross sections weighted by their uncertainties. Thus, the  $c_k$  values represent the systems similarity with respect to materials with the highest sensitivity/uncertainty combination.

## Generalized Linear Least-Squares Methodology

The final procedure utilized in this work is based on the generalized linear least-squares method (GLLSM) introduced by Gandini [11], Dragt et al. [12], and Barhen, Wagschal, and Yeivin [13,14]. The GLLSM has been referred to as a data adjustment procedure, a data consistency analysis, and even a data evaluation technique. The most appropriate description of this particular application would be a generalized trending analysis tool. Physically, the GLLSM is designed to force agreement between the measured and calculated values of  $k_{\text{eff}}$  for the entire set of criticals used in the data validation process. The resulting "data changes" that result from the application of the GLLSM can then be used to predict the biases for *any* similar application where the area of application corresponds to an interpolation or extrapolation scenario.

The derivation of the GLLSM equations in this work follows the general notation from Ref. 15. The vector  $m / (m_i), i = 1, 2, \dots, I$  represents a series of  $k_{\text{eff}}$  measurements on critical benchmark experiments that are to be used in the validation of a dataset for criticality safety computations. This vector  $m$  has a corresponding symmetric  $I \times I$  uncertainty matrix associated with it which we denote as  $C_{mm} / \text{cov}(m_i, m_j) / \langle *m_i *m_j \rangle$ . Further, we denote the vector  $k / (k_i)$  as the corresponding series of calculated values of  $k_{\text{eff}}$  for each of these experiments. The vector  $\mu / (\mu_n), n = 1, 2, \dots, N$ , with its corresponding symmetric  $N \times N$  uncertainty matrix  $C_{\mu\mu} / \text{cov}(\mu_n, \mu_m) / \langle * \mu_n * \mu_m \rangle$ , represents the differential data used in the calculations (i.e., nuclear data, such as fission, capture, and scattering cross sections, the fission spectrum and neutrons per fission quantities) and, additionally, the material densities used in the problem description. This procedure also allows for the possibility of correlations between the integral and differential quantities, which may be present at times in the analysis. These correlations are denoted by the  $N \times I$  covariance matrix  $C_{\mu m} / \langle * \mu_n * m_i \rangle$ .

The sensitivities of the calculated  $k_{\text{eff}}$  to the  $\mu$  parameters are given as  $S_k / \partial k_i / \partial \mu_n$ , with  $S_k$  being an  $I \times N$  matrix. Representing perturbation of the  $\mu$  parameters as linear changes in the calculated  $k_{\text{eff}}$  value, yields the following:

$$k(\mu) = k(\mu + \delta\mu) = k(\mu) + \delta k \cdot k(\mu) + S_k \delta\mu, \quad (1)$$

with the corresponding uncertainty matrix of the calculated values of

$$C_{kk} / \langle *k_i *k_j \rangle = S_k \langle * \mu_n * \mu_m \rangle S_k^T = S_k C_{\mu\mu} S_k^T. \quad (2)$$

If we denote the deviations of the measured responses from their corresponding calculated values by the vector  $d / (d_i) = k(\mu) - m$ , then the uncertainty matrix for the deviation vector  $d$ , denoted by  $C_{dd}$ , is

$$\begin{aligned} C_{dd} &= C_{kk} + C_{mm} - S_k C_{\mu m} - C_{\mu m} S_k^T, \\ &= S_k C_{\mu\mu} S_k^T + C_{mm} - S_k C_{\mu m} - C_{\mu m} S_k^T. \end{aligned} \quad (3)$$

Denoting  $x = \mu - \mu$ , and  $y = m - m = k(\mu) - m$ , we can rewrite Eq. (1) as

$$y = d + S_k x. \quad (4)$$

The measured  $k_{\text{eff}}$  values  $m_i$  and the measured (or evaluated from measurements) parameter values  $\mu_n$  both have their corresponding uncertainties. The best evaluated parameters  $\mu_n$  and the best evaluated  $k_{\text{eff}}$  values  $m_i$  will be those values that are consistent with each other, namely  $m_i = k_i(\mu)$ , and are consistent with their estimated values and uncertainties (i.e., they do not deviate too much from their current best estimates  $m_i$  and  $\mu_n$ , respectively).

The GLLSM procedure involves minimizing the quadratic loss function

$$Q(\mathbf{x}, \mathbf{y}) = (\mathbf{y}, \mathbf{x})^T \begin{pmatrix} C_{mm} & C_{m\alpha} \\ C_{\alpha m} & C_{\alpha\alpha} \end{pmatrix}^{-1} (\mathbf{y}, \mathbf{x}), \quad (5)$$

where  $(\mathbf{y}, \mathbf{x})^T / (y_1, y_2, \dots, y_I, x_1, x_2, \dots, x_N)$ , subject to the constraint expressed by Eq. (4). Adopting the procedure of Refs. 14–16, the above conditional minimum formulation is equivalent to unconditionally minimizing the function  $R(\mathbf{x}, \mathbf{y})$ , where

$$R(\mathbf{x}, \mathbf{y}) = Q(\mathbf{x}, \mathbf{y}) + 2\boldsymbol{\lambda}^T (\mathbf{S}_k \mathbf{x} - \mathbf{y}), \quad (6)$$

and  $2\boldsymbol{\lambda}$  is an  $I$ -dimensional vector of Lagrange multipliers. Thus  $\mathbf{x}$  and  $\mathbf{y}$  satisfy the equations

$$\nabla R(\mathbf{x}, \mathbf{y}) / \nabla \mathbf{x} = \nabla R(\mathbf{x}, \mathbf{y}) / \nabla \mathbf{y} = 0. \quad (7)$$

Solving the resulting equations for  $\mathbf{x}$  and  $\mathbf{y}$ , we obtain

$$\begin{aligned} \mathbf{x} &= \mathbf{m} + (C_{mm} - C_{m\alpha} \mathbf{S}_k^T) C_{dd}^{-1} \mathbf{d}, \text{ and} \\ \mathbf{y} &= \mathbf{m} + (C_{mm} - C_{m\alpha} \mathbf{S}_k^T) C_{dd}^{-1} \mathbf{d}, \end{aligned} \quad (8)$$

where  $C_{dd}^{-1}$  is obtained by taking the inverse of Eq. (3) and is a matrix of dimension  $I \times I$ .

This could of course suggest that any criticality application that is similar to the benchmarks used should be calculated using the modified cross sections and thus have a reduced uncertainty. However, even if we want to stick to “conventional” criticality estimates using “established” cross sections and trend curves, the GLLSM approach can be beneficial, as will be demonstrated in the next section.

In summary, the GLLSM procedure, as applied to the validation of cross-section libraries for criticality safety applications, is designed to predict the data changes,  $\mathbf{x}$ , such that the differences between measured and calculated  $k_{\text{eff}}$  values (i.e., the quantity,  $\mathbf{y}$ ) is minimized. These original  $k_{\text{eff}}$  differences give rise to the trends observed in the trending analyses. Removal of these trends and identification of the data responsible for them is the key to the application of GLLSM techniques to criticality safety data validation.

### ***Application of GLLSM to Data Validation***

The solution of Eq. (8) allows us to evaluate the  $\mathbf{x}$  and  $\mathbf{y}$  quantities in Eq. (4). Of particular interest is the quantity  $\mathbf{d}$  which has been defined as  $(k - m)$ . This quantity is the calculated versus measured discrepancy in  $k_{\text{eff}}$  as determined from the as-specified experimental benchmark description and given cross sections. Rarely do the actual criticality safety scenarios match exactly with one of the experimental benchmarks. Thus, the actual quantity of interest is an estimate of the quantity  $\mathbf{d}$  for the criticality safety scenario of interest, denoted the “application.” In general, the application is an interpolation of the available critical benchmarks, in that it is in the same range or area of applicability with endpoints of the range clearly defined. Occasionally, the application is in the area of applicability, but somewhat outside the endpoints of that area. This situation requires an extrapolation of the available validation data. Both the interpolation and extrapolation situations technically require a so-called translation of the available data, which is traditionally accomplished by trending curves. This translation is accomplished visually by observing significant trends versus trending parameters, (i.e., H/X, EALF, enrichment, etc.) and coverage by observing the density of data points near the application data point.

The systematic application of GLLSM to the interpolation and extrapolation problems described above amounts to a formal procedure for evaluation of the quantity  $\mathbf{d}$  for the applications of interest. Since the

application is assumed to be similar but *not* exactly like one of the experimental benchmarks, the key to the procedure is that we can rewrite Eq. (4) for the application as:

$$k_a(\beta) - m_a = [k_a(\beta) - m_a] + S_a(\beta - \beta_0), \quad (9)$$

where  $S_a$  are the calculated sensitivities for the application. The GLLSM theory predicts that if a sufficient number of experiments are similar to the application of interest, the calculated value of  $k_{\text{eff}}$ , using the “best” cross sections,  $\beta_0$ , will indeed approach the value  $m_a$  and thus, Eq. (9) yields the predicted value of the application bias  $d_a = k_a(\beta) - m_a$  which is obtained when using the given cross sections  $\beta$  as

$$d_a = -S_a(\beta - \beta_0), \quad (10)$$

where  $\beta_0$  was obtained in Eq. (8) using similar benchmark criticality measurements.

### Application of Methodology to Enrichments Above 5 wt %

This current report presents an illustrative application of both the S/U and GLLSM procedures to an area of current interest. The application being studied in this report is the validation of criticality safety studies for facilities processing uranium fuels with enrichments greater than 5 wt %. In the past, these processing facilities have been limited to enrichments at or below 5 wt %. Hence, much of the critical experiment data correspond to these lower enrichments. As a part of this study, a number of critical experiments in the 5–20-wt % range were identified as having been performed in Russia. A number of these experiments were obtained and documented as a result of this work [16].

As with any criticality data validation, the goal is to estimate the bias trends for ranges over which the criticality safety calculational studies are to be performed. The use of S/U and GLLSM methods in validation studies was demonstrated by performing a validation of a hypothetical set of application scenarios, which consist of 14 systems, each having U(11)O<sub>2</sub> fuel with H/X values varying from 0 to 1000. The validation effort included both the traditional trending analyses, trending analysis with the D and  $c_k$  parameters, and finally the full GLLSM approach. Advantages and disadvantages of each approach were explored, and guidance for general use of these techniques was developed.

### Traditional Trending Analysis

In order to clearly show the relationship between the GLLSM techniques and the more traditional techniques for criticality safety validation, a traditional trending analysis using a validation set of 68 benchmark experiments [17] is presented. In Fig. 1,  $k_{\text{eff}}$  is trended versus the energy of average lethargy causing fission (EALF). The prediction from this analysis would be a nearly constant positive bias of about 0.3%. The standard deviations on these bias trends would vary from about 1% for low energies to about 2% at high energies. Trend plots were also generated for H/X and enrichment parameters. The H/X trend plot shows a slight trend, with the predicted  $k$  bias near zero for high H/X values and about + 0.005 for low H/X values. The trend with enrichment is similar, but not enough data are present for the intermediate enrichments to confirm the trend.

It was noted that the largest variations ( $\pm 2\%$ ) about the trend lines were seen for fast systems (i.e., the right-hand portion of the EALF trend plot and the lower portion of the H/X trend plot). Upon examination, it was observed for H/X=0 systems that the predicted  $k_{\text{eff}}$  values less than unity were from the HEUMET set of criticals, while the systems with predicted eigenvalues greater than unity were from the Big-10 and ZPR sets. The combined effects of the high- versus low-enrichments and the processing of the 44GROUPNDF5 library (collapsed using a thermal reactor spectrum) are believed to be responsible for this variation.

As a result of the trending analysis, a prediction of the  $\beta$  k bias and its uncertainty can be obtained for each of the U(11)O<sub>2</sub> systems. Predictions using the USLSTATS [18] procedure for U(11)O<sub>2</sub> systems with H/X values of 0, 3, 40, and 500 are given in Table 1.

### *Trending Analysis using D Values*

This section will discuss trending analyses using the same set of 68 benchmarks as the traditional analyses shown above; however, the trending parameter is now the D coefficients, described earlier. Even though it is possible to perform the trending on each of the D coefficients independently, it was decided to trend  $k_{\text{eff}}$  versus the sum of these coefficients (i.e.,  $D_{\text{sum}}=D_c + D_n + D_s$ ). This method reduces the number of trends plots to be examined.

The trend plot of  $k_{\text{eff}}$  versus  $D_{\text{sum}}$  is given in Fig. 2 for the U(11)O<sub>2</sub> H/X=3 system. These plots are analyzed in quite a different method from the traditional approach. A  $D_{\text{sum}}$  value of zero corresponds to the U(11)O<sub>2</sub> H/X=3 system. The trend line must therefore be extrapolated to zero in order to estimate the  $\beta$  k bias. Therefore, the slope of the trend line is not nearly as important as where it crosses zero and how many systems are in the region of  $D_{\text{sum}}$  less than 1.2. Using these procedures, all cases look like extrapolations, even though not all cases are indeed extrapolations. From this plot it is clear that perhaps only one other system could be considered similar to the U(11)O<sub>2</sub> H/X=3 system (i.e.,  $D_{\text{sum}}$  less than 1.2). Hence, the predicted bias will have somewhat large uncertainties associated with it. The trend plot for the U(11)O<sub>2</sub> H/X=40 system was also generated. Here the coverage near a  $D_{\text{sum}}$  value of zero is much better than that shown in Fig. 2. In this case, there are at least 8 systems with  $D_{\text{sum}}$  values of 1.2 or less. The trend plot for the last system (i.e., U(11)O<sub>2</sub> H/X=500) gives conclusions that are very similar to those for the H/X=40 example. There are a large number of systems within a  $D_{\text{sum}}$  value of 1.2, with a resulting good prediction of the  $\beta$  k bias for this system.

These trending analysis results are generated using the same software that was used in the traditional trending approach previously [see Ref. 18]. Therefore, the same estimates of the  $\beta$  k bias and its uncertainty can be obtained from these analyses. These bias predictions are given in Table 1.

### *Trending Analysis using $c_k$ Values*

The trending analyses using the  $c_k$  values follows very closely to the analyses using the D coefficients discussed in the previous section. Here the trend curves are interpreted as an extrapolation to a  $c_k$  value of unity, which corresponds to the particular application system of interest. The slope of the trend curve is again of secondary importance; the items of primary importance are the number of systems with a  $c_k$  value greater than 0.8 and the value of the predicted  $\beta$  k bias at a  $c_k$  value of unity.

The  $k_{\text{eff}}$  trend plot for  $c_k$  of a U(11)O<sub>2</sub> H/X=0 system is shown in Fig. 3. This trend plot is interesting when compared with the traditional trend plot shown in Fig. 1. The four data points in the upper-right-hand portion of both plots correspond to the same four systems (three ZPR and Big-10 systems). In Fig. 1, the predicted  $\beta$  k bias is about 0.4% because the overprediction of  $k_{\text{eff}}$  for these four systems is counteracted by the underprediction of the HEUMET systems which all have very similar values of EALF. However, the trend seen for  $k_{\text{eff}}$  in Fig. 3 is caused by the lack of similarity between the U(11)O<sub>2</sub> H/X=0 and HEUMET systems. These HEUMET systems can be seen in Fig. 3 with a  $c_k$  value of about 0.5–0.6, indicating only minor correlations with the U(11)O<sub>2</sub> H/X=0 system. This example shows the potential improvement from the use of a trending analysis with these new parameters, since trends can be observed as a function of systems that are expressly determined to be similar. It is clear from the preceding analyses that sometimes the traditional parameters indicate that systems should be similar, but are not. In this particular case, the predicted bias is much larger than that predicted by the standard techniques.

The trend plots for the remaining U(11)O<sub>2</sub> systems with H/X values of 3, 40, and 500 were also studied using the  $c_k$  values. For the systems with H/X values of 3 and 40, the predicted biases are higher than those predicted by the standard techniques. The specific reasons for these differences were not explored in depth as with the H/X of 0 cases, but are believed to be caused by the separation of effects that tended to cancel each other. The  $k$  bias predicted for the H/X=500 system are in line with those of the standard techniques since a large number of experiments are considered to be similar, and no cancellation of effects is seen.

These trending analysis results are generated using the same software that was used previously. Estimates of the  $k$  bias and its uncertainty from this trending approach are given in Table 1.

Table 1: Comparison of predicted  $k$  bias and its standard deviation<sup>a</sup> for various procedures

Procedure	H/X=0		H/X=3		H/X=40		H/X=500	
	bias (%)	std. dev. (%)						
EALF	0.32	0.74	0.45	0.74	0.46	0.74	0.46	0.74
H/X	0.49	0.77	0.49	0.77	0.47	0.77	0.31	0.77
D <sub>sum</sub>	-	-	1.26	0.76	0.66	0.78	0.28	0.78
$c_k$	1.28	0.73	1.40	0.69	0.69	0.76	0.39	0.78
GLLSM	2.56	0.38	1.30	0.33	0.77	0.40	0.63	0.37

<sup>a</sup>For all but GLLSM, the standard deviations correspond to the “pooled standard deviation” as specified in Ref. 18 because this definition was judged to best match that provided by GLLSM.

## Summary

In the preceding sections, results from a number of approaches to criticality safety data validation were presented. The GLLSM results shown in Table 1 were taken directly from Ref. 17. Quite interestingly, they give very different answers for the set of application problems chosen for study. The primary reason for these differences seems to be the inclusion of systems that may “look” very similar from the standpoint of certain parameters, but very different with respect to other parameters. In particular, according to both the H/X and EALF parameters, both the HEUMET and ZPR/Big-10 problems are similar. However, with respect to the sensitivities and uncertainties, they appear to be quite different. Cancellation of effects due to systems that “appear” to be similar causes the *traditional trending approaches to underpredict the actual bias for low-moderation systems with intermediate enrichments*. This is evident in Table 1, where the results are presented in summary form. The predicted bias from these applications are all positive (overpredict  $k_{eff}$ ). Therefore, the variation in results is not a concern for these applications. However, a similar situation can be easily postulated where a predicted positive bias is actually a negative bias. With the inclusion of strict confidence levels along with an additional margin of subcriticality, the cumulative effect of these factors should still be conservative. However, *prudent application of trending procedures is very important in criticality safety validation exercises*.

These new criticality safety data validation procedures discussed in this paper appear to be useful for a wide variety of application areas. The advantage of these procedures is that the determination of similar systems is automatic because the systems are trended with the D and  $c_k$  values. Also, the inclusion of a wide variety of benchmarks in the validation set is possible, since the trending parameters will selectively fit only systems that are similar to the particular application area. Further guidance on the use of these new techniques is given in Ref. 17.

## Acknowledgments

The authors are grateful to the U.S. Nuclear Regulatory Commission for their sponsorship of the work described in this paper.

## References

1. E. M. Oblow, "Sensitivity Theory from a Differential Viewpoint," *Nucl. Sci. Eng.*, **59**, 187 (1976).
2. W. M. Stacey, Jr., "Variational Estimates and generalized Perturbation Theory for the Ratios of Linear and Bilinear Functionals," *J. Math. Phys.*, **13**, 1119 (1972); see also; W. M. Stacey, Jr., "Variational Estimates of Reactivity Worths and Reaction Rate Ratios in Critical Nuclear Reactors," *Nucl. Sci. Eng.*, **48**, 444 (1972).
3. L. N. Usachev, "Perturbation Theory for the Breeding Ratio and for Other Number Ratios Pertaining to Various Reactor Processes," *J. Nucl. Energy*, Pts. A/B, **18**, 571 (1964).
4. A. Gandini, "A Generalized Perturbation Method for Bilinear Functionals of the Real and Adjoint Neutron Fluxes," *J. Nucl. Energy*, **21**, 755 (1967).
5. B. L. Broadhead, R. L. Childs, and B. T. Rearden, "Computational Methods for Sensitivity and Uncertainty Analysis in Criticality Safety," *Proceedings of ICNC'99 Sixth International Conference on Nuclear Criticality*, September 20–24, 1999, Paris, France (1999).
6. J. L. Lucius, C. R. Weisbin, J. H. Marable, J. D. Drischler, R. Q. Wright, and J. E. White, "A Users Manual for the FORSS Sensitivity and Uncertainty Analysis Code System," ORNL-5316, Union Carbide Corporation, Oak Ridge National Laboratory, January 1981.
7. O. W. Hermann and R. M. Westfall, "ORIGEN-S: SCALE System Module to Calculate Fuel Depletion, Actinide Transmutation, Fission Product Buildup and Decay, and Associated Radiation Source Terms," Vol. II, Sect. F7 of *SCALE - A Modular Code System for Performing Standardized Computer Analysis for Licensing Evaluation*, NUREG/CR-0200, Rev. 4 (ORNL/NUREG/CSD-2/R4), March 1995. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.
8. R. L. Childs, "SEN1: A One-Dimensional Cross-Section Sensitivity and Uncertainty Module for Criticality Safety Analysis," NUREG/CR-5719 (ORNL/TM-13738), U.S. Nuclear Regulatory Commission, in preparation.
9. J. D. Smith, III and B. L. Broadhead, "Multigroup Covariance Matrices for Fast Reactor Studies," ORNL/TM-7389, Union Carbide Corporation, Oak Ridge National Laboratory, 1981.
10. R. E. McFarlane, R. J. Barrett, D. W. Muir, and R. M. Boicourt, "The NJOY Nuclear Data Processing System: User's Manual," LA-7584-M, Los Alamos National Laboratory, 1978.
11. A. Gandini, "Nuclear Data and Integral Measurements Correlation for Fast Reactors, Part 1: Statistical Formulation," RT/FI(73)5, Comitato Nazionale Energia Nucleare (1973).
12. J. B. Dragt, J. W. M. Dekker, H. Gruppelaar, and A. J. Janssen, "Methods of Adjustment and Error Evaluation of Neutron Capture Cross Sections; Application to Fission Product Nuclides," *Nucl. Sci. Eng.*, **62**, 117 (1977).

13. J. J. Wagschal, and Y. Yeivin, "The Significance of Lagrange Multipliers in Cross-Section Adjustment," *Trans. Am. Nucl. Soc.*, **34**, 776 (1980).
14. J. Barhen, J. J. Wagschal, and Y. Yeivin, "Response-Parameter Correlations in Uncertainty Analysis," *Trans. Am. Nucl. Soc.*, **35** (1980).
15. R. E. Maerker, B. L. Broadhead, and J. J. Wagschal, "Theory of a New Unfolding Procedure in Pressurized Water Reactor Pressure Vessel Dosimetry and Development of an Associated Benchmark Data Base," *Nucl. Sci. Eng.*, **91**, 369 (1985). See also "Development and Demonstration of an Advanced Methodology for LWR Dosimetry Applications," EPRI NP-2188, Electric Power Research Institute, Palo Alto, California, December 1981.
16. B. T. Rearden, J. J. Lichtenwalter, and C. M. Hopper, "Evaluation of Critical Experiment Parameters and Uncertainties With First-Order Sensitivity Techniques," NUREG/CR-5624 (ORNL/TM-13718), U.S. Nuclear Regulatory Commission, in preparation.
17. B. L. Broadhead, C. M. Hopper, and C. V. Parks, "Sensitivity and Uncertainty Analyses Applied to Criticality Validation, Volume 2: Illustrative Applications and Initial Guidance," NUREG/CR-5593, Vol. 2 (ORNL/TM-13693/V2), U.S. Nuclear Regulatory Commission, in preparation.
18. J. J. Lichtenwalter, S. M. Bowman, M. D. DeHart, and C. M. Hopper, *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages*, Appendix C, "User's Manual for USLSTATS V1.0," pp. 339–344, NUREG/CR-6361 (ORNL/TM-13211), U.S. Nuclear Regulatory Commission, March 1997.

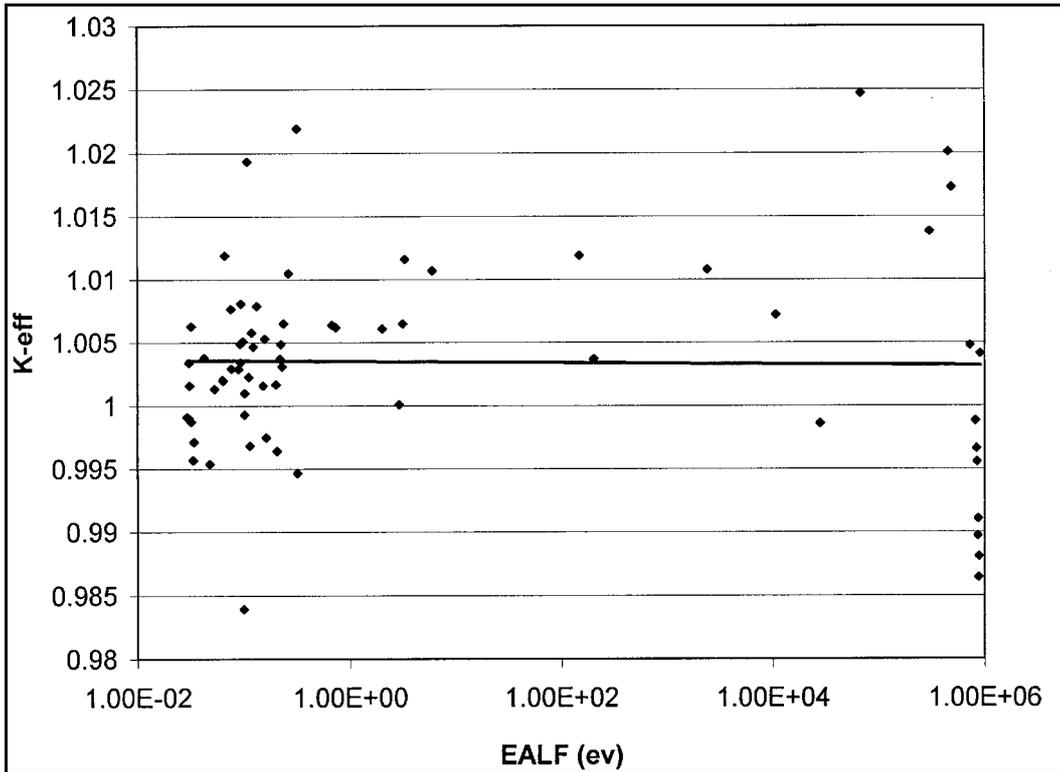


Figure 1. Trend plot for  $k_{\text{eff}}$  versus energy of average lethargy causing fission (EALF).

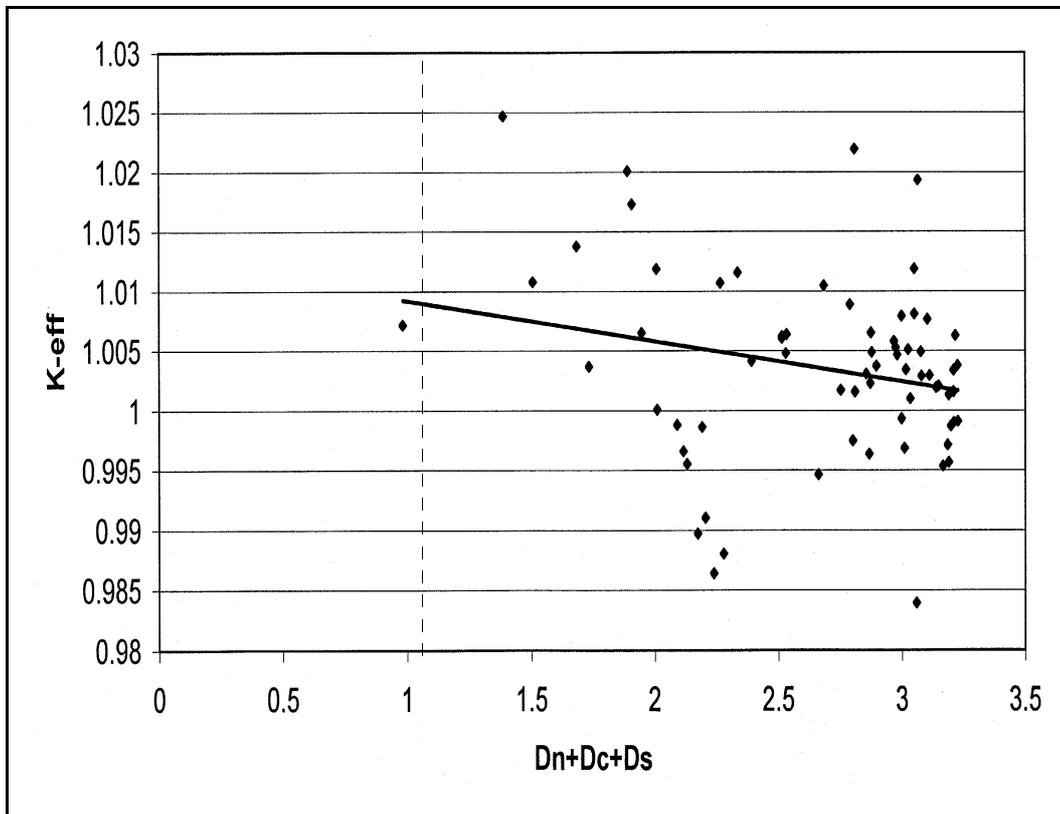


Figure 2. Trend plot for  $k_{\text{eff}}$  versus  $D_{\text{sum}}$  value for the  $\text{U}(11)\text{O}_2$   $\text{H}/\text{X}=3$  system.

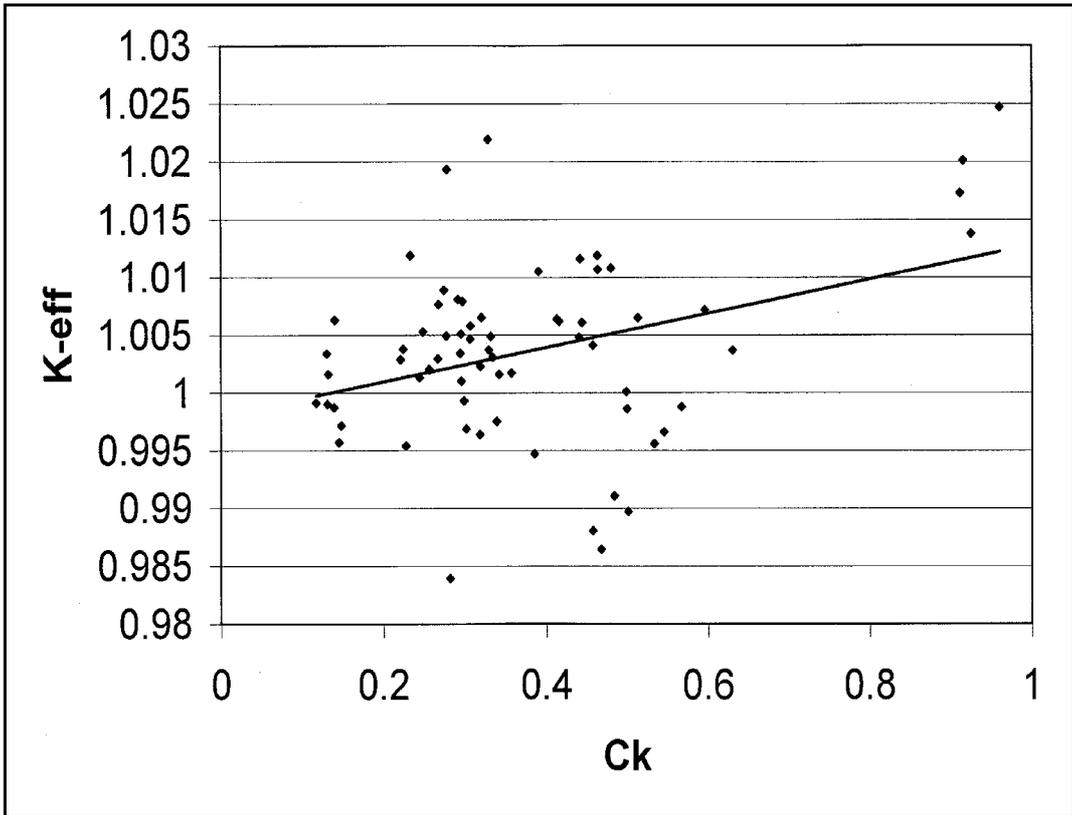


Figure 3. Trend plot for  $k_{\text{eff}}$  versus  $c_k$  value for the U(11)O<sub>2</sub> H/X=0 system.

