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B. L. Broadhead, R. L. Childs and C. M. Hopper

Oak Ridge National Laboratory,*
P. O. Box 2008,
Oak Ridge, TN 37831-6370
(865) 576-4476

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1. Introduction

The first two papers in this series[1,2] have described Sensitivity and Uncertainty (S/U) Theory for application to criticality safety validation exercises. Those papers describe the use of S/U methods to select and define benchmarks that are applicable to a particular application area. Each of these methods define parameters that are useful in traditional trending analyses that establish predicted computation/nuclear data biases as well as upper subcritical limits. This paper will describe a generalized linear least squares methodology (GLLSM) that can also be used to establish computational/nuclear data biases. Subsequently, each of these methods will be used in an illustrative application with the results of these new techniques compared with those of typical criticality safety trending analyses.

The GLLSM procedure is an alternative approach to the traditional trending analysis for the determination of biases. The inputs 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 actual 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 benchmark area of applicability.

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One of the benefits of the GLLSM approach is that, not only can the bias for a given application be estimated, the cumulative "combination" of critical benchmarks can be used to determine the convergence of the procedure. Questions that can be addressed include: how many experiments are needed to verify an application, and how much correlation to the application is necessary in order to validate the application area?

Previously,[3] the GLLSM was used to predict how many experiments and how much correlation between experiments is necessary to validate an application area. In this paper, the GLLSM is applied as a data validation tool for comparison with the traditional trending analyses and trending versus E and c_k[1] parameters.

This paper presents an illustrative application of both the S/U and GLLSM methods to the validation of criticality safety studies for facilities processing uranium fuels with enrichments greater than 5 wt % for use in commercial power reactors. 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 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 usefulness 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 $U(11)O_2$ fuel with H/X values varying from 0 to 1000. The 11 wt % enrichment was chosen so the entire range of moderation conditions, including dry, could be studied. The data validation included traditional trending analyses, trending analyses with the E and c_k parameters, and finally the full GLLSM approach. Advantages and disadvantages of each approach are explored, and guidance for general use of these techniques is developed.

2. GLLSM Theory

The procedures utilized in this work are based on the generalized linear-least-squares method described in Ref. 4. 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 GLLSM for this particular application would be that of a generalized trending analysis tool. Physically the GLLSM is designed to force agreement between the measured and calculated values of k_{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 (via interpolation or extrapolation) the biases for *any* application determined to be similar to the benchmark area of applicability. Functionally, the GLLSM can be thought of as a trending of a suite of critical benchmarks with respect to the cross-section correlation coefficient between the various systems. The GLLSM has the capability to identify experiments that contain inconsistencies (i.e., the magnitude of the measured-to-calculated k_{eff} difference is larger than their combined uncertainties). A chi-squared consistency indicator is used to directly predict the overall consistency of the suite of benchmarks. A chi-squared value for each experiment is also available from the GLLSM method.

The derivation of the GLLSM equations in this work follows the general notation from Ref. 3. The vector $m \equiv (m_i)$, $i = 1, 2, \ldots I$, represents a series of k_{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 is denoted as $C_{mm} \equiv \mathrm{cov}(m_i,m_j) \equiv \langle \delta m_i \delta m_j \rangle$. Further, the vector $k \equiv (k_i)$ is denoted as the corresponding series of calculated values of k_{eff} for each of these experiments. The vector $\alpha \equiv (\alpha_n)$, $n = 1, 2, \ldots N$, with its corresponding symmetric $N \times N$ uncertainty matrix $C_{\alpha\alpha} \equiv \mathrm{cov}(\alpha_n \alpha_m) \equiv \langle \delta\alpha_n \delta\alpha_m \rangle$, 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 $C_{\alpha m} \equiv \langle \delta\alpha_n \delta m_i \rangle$.

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

$$k(\alpha') = k(\alpha + \delta\alpha) = k(\alpha) + \delta k \simeq k(\alpha) + S_k \delta\alpha \ , \tag{1}$$

with the corresponding uncertainty matrix of the calculated values of

$$C_{kk} \equiv \langle \delta k_j \delta k_j \rangle = S_k \langle \delta\alpha_n \delta\alpha_m \rangle S_k = S_k C_{\alpha\alpha} S_k^H \ . \tag{2}$$

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

$$\begin{aligned} C_{dd} &= C_{kk} + C_{mm} - S_k C_{\alpha m} - C_{m\alpha} S_k^H \ , \\ &= S_k C_{\alpha\alpha} S_k^H + C_{mm} - S_k C_{\alpha m} - C_{m\alpha} S_k^H \ . \end{aligned} \tag{3}$$

Denoting $x = \alpha' - \alpha$, and $y = m' - m = k(\alpha') - m$, we can rewrite Eq. (10) as

$$y = d + S_k x \ . \tag{4}$$

The measured k_{eff} values, m_i, and the measured (or evaluated from measurements) parameter values, α_n, both have their corresponding uncertainties. The best evaluated parameters α_n' and the best evaluated k_{eff} values m_i' will be those values that are consistent with each other, namely $m_i' = k_i(\alpha'_n)$, 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 α_n, respectively).

The GLLSM procedure involves minimizing the quadratic loss function

$$Q(x,y) = (y,x)^{\mathsf{H}} \begin{pmatrix} C_{mm} C_{m\alpha} \\ C_{\alpha m} C_{\alpha\alpha} \end{pmatrix}^{-1} (y,x) \ , \tag{5}$$

where $(y,x)^{\dagger} \equiv (y_1, y_2, ..., y_I, x_1, x_2, ..., x_N)$, subject to the constraint expressed by Eq. (4). Adopting the procedure of Ref. 3, the above conditional minimum formulation is equivalent to unconditionally minimizing the function $R(x,y)$, where

$$R(x,y) = Q(x,y) + 2\lambda^{\mathsf{H}}(S_k x - y) \ , \tag{6}$$

and 2λ is an I-dimensional vector of Lagrange multipliers. Thus x and y satisfy the equations

$$\partial R(x,y)/\partial x = \partial R(x,y)/\partial y = 0 \ . \tag{7}$$

Solving the resulting equations for x and y, we obtain

$$\begin{aligned} \alpha' &= \alpha + (C_{\alpha m} - C_{\alpha\alpha} S_k^{\mathsf{H}}) C_{dd}^{-1} d, \text{ and} \\ m' &= m + (C_{mm} - C_{m\alpha} S_k^{\mathsf{H}}) C_{dd}^{-1} d, \end{aligned} \tag{8}$$

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

A few observations are due here:

1. If the α' values obtained in Eq. (8) are substituted in $k(\alpha')$, using the linearity assumption of Eq. (1), the m' value of Eq. (8) is obtained, thus $m' = k(\alpha')$ is satisfied.
2. Moreover, not only are the new/best estimates of the cross sections and of the k_{eff} values consistent, but their uncertainties are reduced as well.

These reduced uncertainties are given by

$$C_{m'm'} = C_{mm} - C_{yy} \text{ and } C_{\alpha'\alpha'} = C_{\alpha\alpha} - C_{xx} \ , \tag{9}$$

where

$$\begin{aligned} C_{yy} &= (C_{mm} - C_{m\alpha} S_k^{\mathsf{H}}) C_{dd}^{-1} (C_{mm} - S_k C_{\alpha m}) \\ C_{xx} &= (C_{\alpha m} - C_{\alpha\alpha} S_k^{\mathsf{H}}) C_{dd}^{-1} (C_{m\alpha} - S_k C_{\alpha\alpha}) \ . \end{aligned} \tag{10}$$

This could of course suggest that any criticality application that is similar to the selected benchmarks should be calculated using the modified cross sections and thus have a reduced uncertainty. However, even when maintaining "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, x, such that the differences between measured and calculated k_{eff} values (i.e., the quantity, y) are minimized. These k_{eff} differences are the trends observed in the traditional criticality safety trending analyses. Removal of these trends and the identification of the data responsible for them are keys to the application of GLLSM techniques to criticality safety data validation.

2.1 Application of GLLSM to Data Validation

The solution of Eq. (8) allows evaluation of the x and y quantities in Eq. (4). Of particular interest is the quantity d, which has been defined as (k - m). This quantity is the calculated-versus-measured discrepancy in k_{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 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 near 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 hydrogen-to-fissile ratio (H/X), energy of average

lethargy causing fission (EALF), enrichment, etc.; coverage is assessed 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 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:

$$k_a(\alpha') - m_a' = [k_a(\alpha) - m_a'] + S_a(\alpha' - \alpha) \ , \tag{11}$$

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_{eff}, using the "best" cross sections, α', will indeed approach the value m_a' and thus, Eq. (11) yields the predicted value of the application bias $d_a = k_a(\alpha) - m_a'$, which is obtained when using the given cross sections α as

$$d_a \simeq -S_a(\alpha' - \alpha) \ , \tag{12}$$

where $\alpha' - \alpha$ was obtained in Eq. (8) using all similar benchmark criticality measurements.

The definitions of "similar" and "sufficient" number of experiments are determined by tests using actual benchmark experiments.

3. S/U and GLLSM ANALYSIS EXAMPLES

The GLLSM methodology as described above is very different from the traditional criticality safety approaches. As an aid to the understanding of this new procedure, this section proceeds through a criticality validation exercise using standard techniques, S/U techniques, and GLLSM techniques as demonstration exercises.

3.1 Description of $U(11)O_2$ Systems

The illustrative application for validation is a series of $U(11)O_2$ systems with H/X values of 0, 3, 5, 10, 20, 40, 80, 200, 300, 400, 500, 600, 800, and 1000. These $U(11)O_2$ systems are "artificial" critical bare spheres generated for calculational comparison purposes. The object of this demonstration problem is the validation of the underlying cross sections and criticality code for these 14 systems.

The dimensions for the $U(11)O_2$ systems were generated via a critical radius search calculation. The critical radii corresponding to the 14 unreflected systems for H/X of 0 to 1000 were 50.55, 40.00, 36.85, 31.77, 26.48, 22.34, 19.87, 18.99, 19.53, 20.39, 21.42, 22.51, 25.41, and 29.17 cm.

3.1.1 Traditional Trending Analysis

In order to clearly show the relationship between the GLLSM techniques and the more traditional techniques for criticality safety validations, a traditional trending analysis using the 102 benchmark experiments described in Ref. 4 is presented. In Figure 1, k_{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%. Similar results were obtained when trended versus H/X (see Ref. 4 for details).

3.1.2 Trending Analysis Using c_k and E Values

In this section, trending analyses using the same set of 102 benchmarks as the traditional analyses shown above are discussed; however, the trending parameters are now the E and c_k coefficients, described in Refs. 1 and 2. Even though it is possible to perform the trending on each of the E coefficients independently, it was decided to trend k_{eff} versus the sum of these coefficients (i.e., $E_{sum} = E_c + E_f + E_s$). This combination reduces the number of trend plots to be examined.

The trend plot of k_{eff} versus E_{sum} is given in Figure 2 for the $U(11)O_2$ H/X=3 system.* These plots are analyzed with a different method from the traditional approach. Here the trend curves are interpreted as an extrapolation to E and c_k values of unity, which correspond to the particular application system of interest. The slope of the trend curve is of secondary importance. The items of primary importance are the number of systems with E and c_k values greater than 0.8 (see refs. 1 and 4) and the value of the predicted Δk bias for E and c_k values of unity.

These trending analysis results are generated using the similar procedures to those used in the traditional trending approach of Section 3.1.1. Therefore, the same type of estimates for the Δk bias and its uncertainty can be obtained from these analyses. These bias predictions are given in Table 1.

3.1.3 GLLSM Analysis of 11 wt % Systems

The GLLSM technique is a procedure completely different from the preceding trending techniques. It does have the same intended endpoint: the determination of the predicted Δk bias for the set of $U(11)O_2$ systems. As was shown in Section 2 of this paper, the GLLSM procedure is capable of

*The $U(11)O_2$ H/X = 0 system was analyzed, but the trend plot is not shown. See Table 1 for a summary of the complete results.

indicating not only the predicted Δk bias, but its uncertainty as well. The result of the application of GLLSM to this set of problems is also shown in Table 1.

Table 1 Comparison of predicted Δk bias and its standard deviation for various procedures

Procedure	H/X = 0		H/X = 3		H/X = 40		H/X = 500	
	% bias	% std. dev.	% bias	% std. dev.	% bias	% std. dev.	% bias	% std. dev.
EALF	0.17	0.70	0.26	0.70	0.26	0.70	0.26	0.70
H/X	0.32	0.71	0.32	0.71	0.31	0.71	0.17	0.71
E_{sum}	0.65	0.71	0.99	0.69	0.25	0.72	0.15	0.71
c_k	1.34	0.66	1.15	0.66	0.26	0.72	0.39	0.79
GLLSM	3.08	0.38	2.11	0.33	0.54	0.40	0.76	0.37

3.2 Summary of Trending Analyses

In the preceding sections, results from a number of approaches to criticality safety data validation were presented. 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[4] and ZPR/Big-10[4] 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 situation is evident in Table 1, where each of the previously reported results is presented in summary form. The predicted biases from these applications are all positive.

Therefore, their overprediction 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.

4. References

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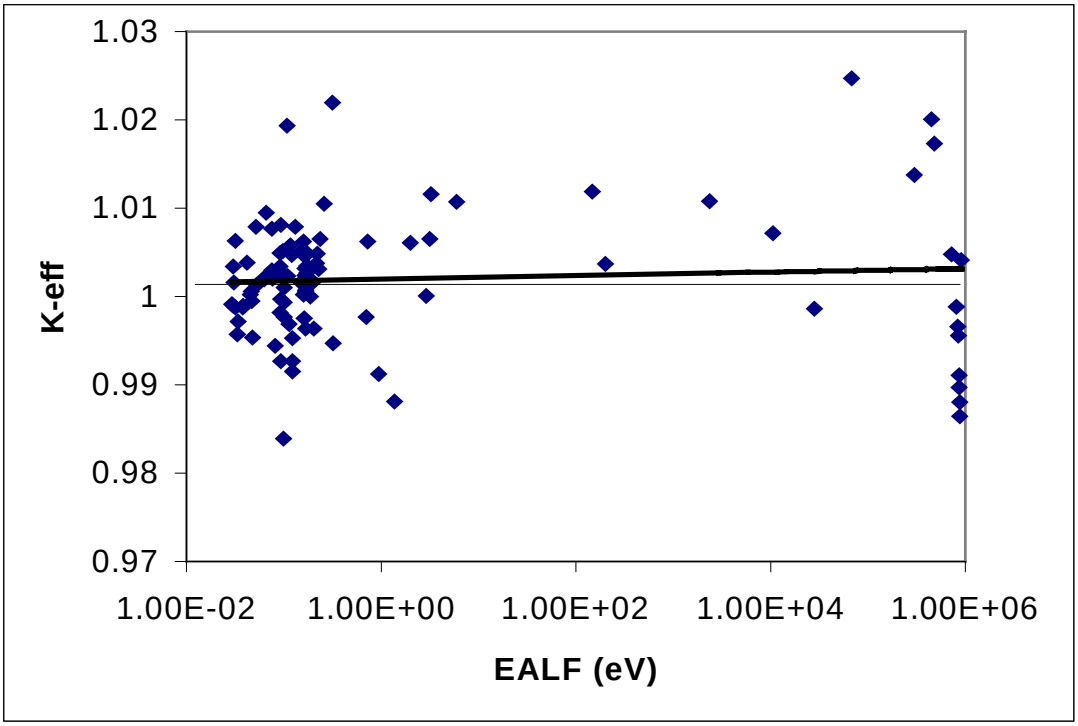

Figure 1. Trend plot of k-eff versus EALF

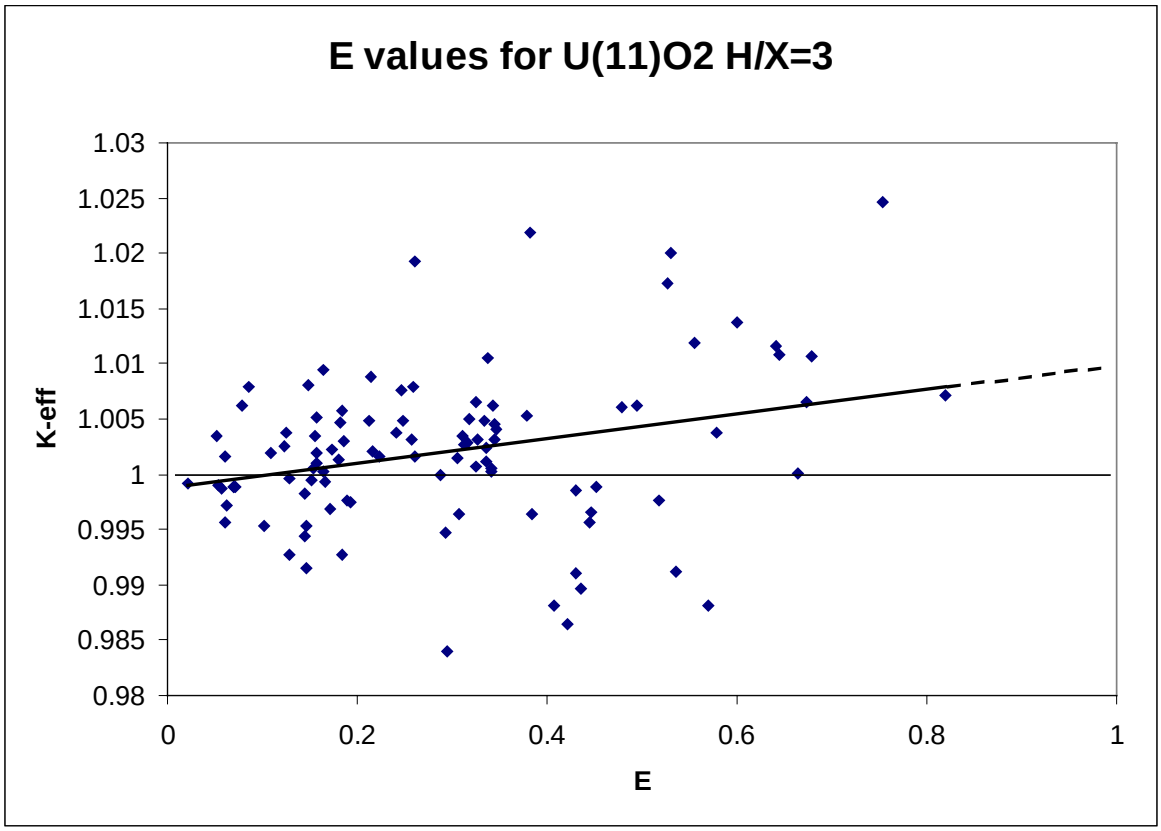

Figure 2. Trend plot of k-eff with E values