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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

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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_{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_{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}U fission, scatter, Σ , 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:

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

where S is the sensitivity of k_{eff} for the safety application, a, or experimental configuration, e, to the capture and scattering cross sections, or to Σ (c, s, or 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_{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_{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_{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_{eff} values, with the addition of an estimate of the uncertainty in the measured k_{eff} values. Mathematically the GLLSM represents a combination of measurements. These measurements include the experimental values of k_{eff} for each critical benchmark and the calculated value of k_{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_{eff} sensitivities, the reader is referred to the accompanying paper [5].

The k_{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_{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_{\dots} and the sensitivity matrices relating changes in each constituent material and process to the system k_{eff} as S_k , the uncertainty matrix for the system k_{eff} values, C_{kk} is given as:

$$C_{kk} = S_k C_{\dots} S_k^T.$$

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_{\dots} matrix is an $N \times N$ matrix, with the resulting C_{kk} matrix $I \times I$. The C_{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_{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_{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 $C_{\text{mm}} / \text{cov}(m_i, m_j) / \langle m_i m_j \rangle$. Further, we denote the vector $k / (k_i)$ as the corresponding series of calculated values of k_{eff} for each of these experiments. The vector $" / ("_n)$, $n = 1, 2, \dots, N$, with its corresponding symmetric $N \times N$ uncertainty matrix $C_{\text{""}} / \text{cov}("_n, "_m) / \langle " _n " _m \rangle$, 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 $C_{\text{""m}} / \langle " _n m_i \rangle$.

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

$$k(" \text{ll}) = k(" + " ") = k(") + " k \bullet k(") + S_k " ", \quad (1)$$

with the corresponding uncertainty matrix of the calculated values of

$$C_{\text{kk}} / \langle k_i k_j \rangle = S_k \langle " _n " _m \rangle S_k^T = S_k C_{\text{""}} S_k^T. \quad (2)$$

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

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

Denoting $x = " \text{ll} - "$, and $y = m \text{ll} - m = k(" \text{ll}) - m$, we can rewrite Eq. (1) as

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

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

The GLLSM procedure involves minimizing the quadratic loss function

$$Q(x,y) = (y,x)^T \begin{pmatrix} C_{mm} & C_{m''} \\ C_{m''} & C_{''} \end{pmatrix} \&l (y,x), \quad (5)$$

where $(y,x)^T / (y_1, y_2, \dots, y_I, x_1, x_2, \dots, x_N)$, 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 $R(x,y)$, where

$$R(x,y) = Q(x,y) + 2\delta^T(S_k x - y), \quad (6)$$

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

$$MR(x,y)/Mx = MR(x,y)/My = 0. \quad (7)$$

Solving the resulting equations for x and y , we obtain

$$\begin{aligned} n &= n + (C_{m''} - C_{''} S_k^T C_{dd}^{-1} d), \text{ and} \\ m &= m + (C_{mm} - C_{m''} S_k^T) C_{dd}^{-1} d, \end{aligned} \quad (8)$$

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

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:

$$k_a("N) - m_aN = [k_a(") - m_aN] + S_a("N - ") , \quad (9)$$

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_{eff} , using the “best” cross sections, “”, will indeed approach the value m_aN , and thus, Eq. (9) yields the predicted value of the application bias $d_a = k_a(") - m_aN$, which is obtained when using the given cross sections “ as

$$d_a \bullet -S_a("N - ") , \quad (10)$$

where “N - ” 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 f

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 β k bias and its uncertainty can be obtained for each of the U(11)O₂ systems. Predictions using the USLSTATS [18] procedure for U(11)O₂ 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_{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_{eff} versus D_{sum} is given in Fig. 2 for the U(11)O₂ H/X=3 system. These plots are analyzed in quite a different method from the traditional approach. A D_{sum} value of zero corresponds to the U(11)O₂ H/X=3 system. The trend line must therefore be extrapolated to zero in order to estimate the β 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_{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)O₂ H/X=3 system (i.e., D_{sum} less than 1.2). Hence, the predicted bias will have somewhat large uncertainties associated with it. The trend plot for the U(11)O₂ H/X=40 system was also generated. Here the coverage near a D_{sum} value of zero is much better than that shown in Fig. 2. In this case, there are at least 8 systems with D_{sum} values of 1.2 or less. The trend plot for the last system (i.e., U(11)O₂ 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_{sum} value of 1.2, with a resulting good prediction of the β 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 β 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 β k bias at a c_k value of unity.

The k_{eff} trend plot for c_k of a U(11)O₂ 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 β k bias is about 0.4% because the overprediction of k

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)O₂ 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^a 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 _{sum}	-	-	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

^aFor 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.

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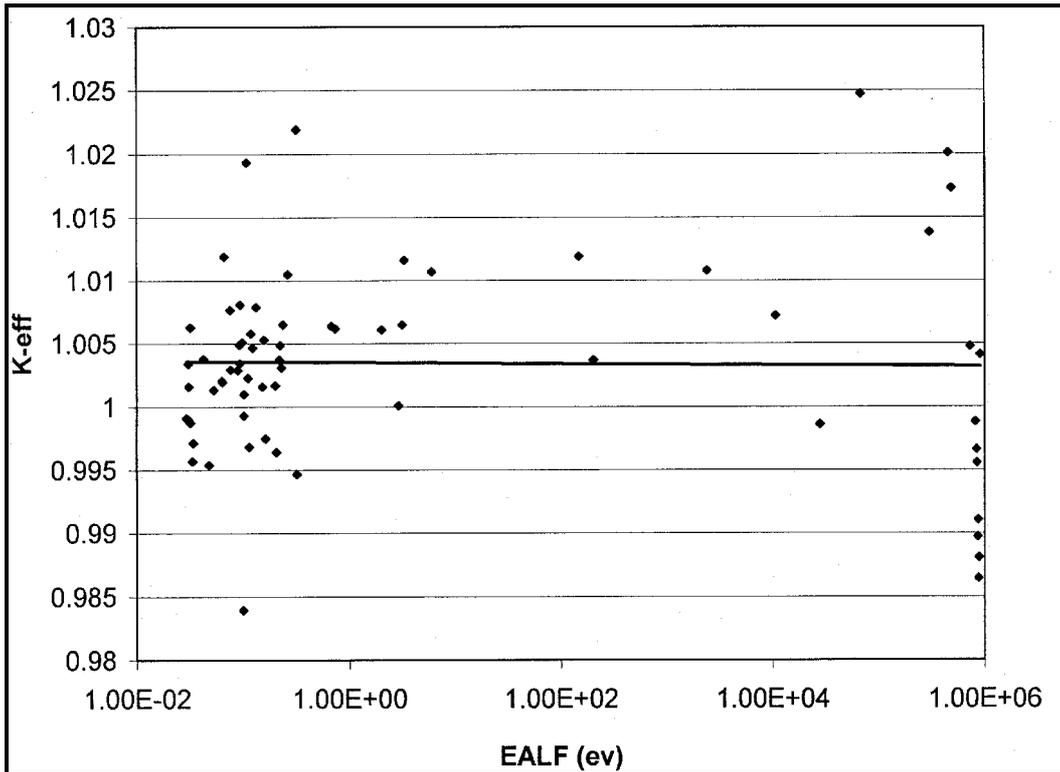


Figure 1. Trend plot for k_{eff} versus energy of average lethargy causing fission (EALF).

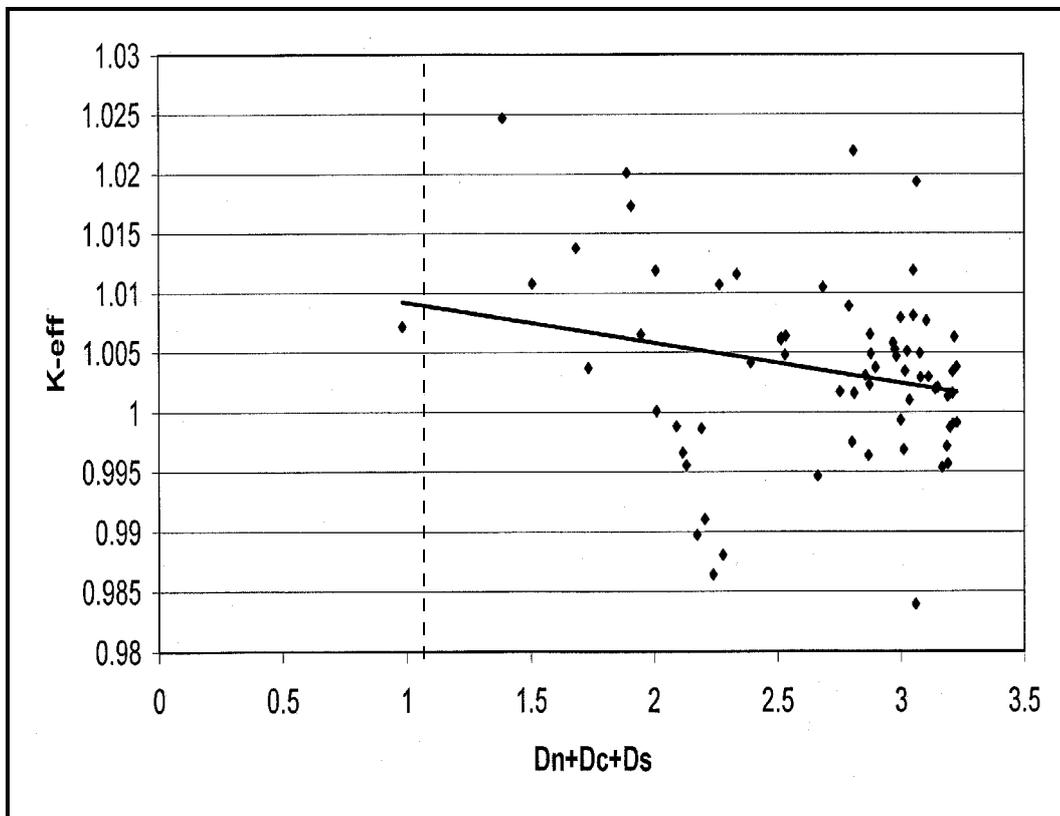


Figure 2. Trend plot for k_{eff} versus D_{sum} value for the $\text{U}(11)\text{O}_2$ $\text{H}/\text{X}=3$ system.

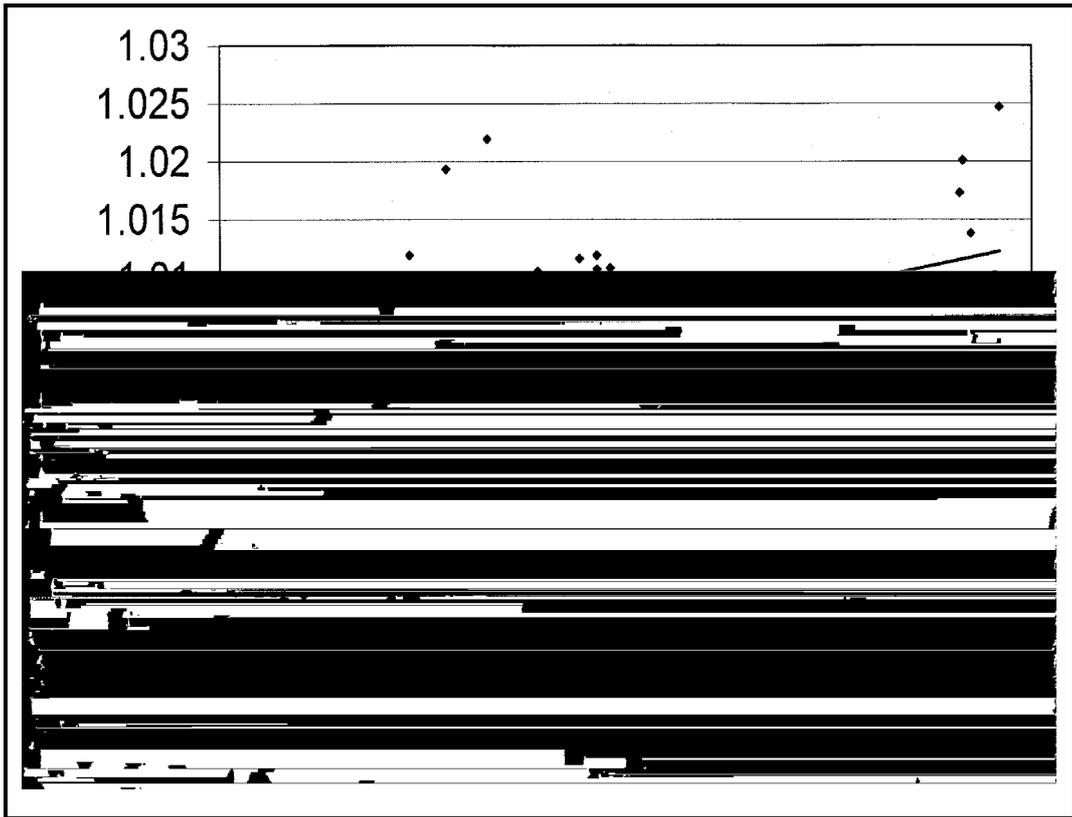


Figure 3. Trend plot for k_{eff} versus c_k value for the U(11)O₂ H/X=0 system.