Journal of ASTM International, Vol. 3, No. 7
Paper ID JAI13461
Available online at www.astm.org

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Generalized Linear Least-Squares Adjustment, Revisited

ABSTRACT: TSURFER, a generalized linear least-squares (GLLS) code, is a new module of the SCALE system. After a short introduction outlining the history and applications of the GLLS methodology in reactor physics, a new application of the GLLS methodology in criticality safety is discussed. Some characteristic TSURFER input data are discussed in detail.

KEYWORDS: TSURFER, SCALE, GLLS, adjustment, uncertainties, LEPRICON, inconsistency, rejection, ENDF/B, ICSBEP

Introduction

Twenty-five years has passed since the Least-Square EPRI Consolidation (LEPRICON) methodology [1] was first proposed for the adjustment of pressure vessel fluence estimates by consolidating neutron transport calculations and surveillance dosimetry measurements. The generalized linear least-squares (GLLS) method has since been recognized as a comprehensive and technically correct approach to the analysis of reactor dosimetry data. The crux of the LEPRICON methodology is the simultaneous adjustment of (a) dosimetry measurements in benchmark fields, (b) surveillance dosimetry measurements in the reactor field under test, (c) dosimetry cross sections, and (d) transport-calculation parameters. This procedure results in the adjustment not only of the fluence *at the surveillance position* but also of the calculated fluence at any point *within the vessel steel*, in particular at the point of estimated maximum damage to the pressure vessel. The GLLS procedure also provides a rigorous estimate for the response uncertainties. This is of particular importance since the latest U.S. Nuclear Regulatory Commission (NRC) regulatory guide [2] emphasizes the need for uncertainty analysis in vessel fluence computations, although there is no well-defined rigorous approach specified for the analysis.

In order to perform the adjustment, each measured quantity must be accompanied by the corresponding calculated value, the experimental uncertainty, and possible correlations with other measured quantities. Uncertainty matrices associated with the dosimetry cross sections as well as with the transport-calculation parameters are also needed. Such a procedure also necessitates the calculation of the sensitivity profiles of the calculated fluences to the transport parameters at the surveillance position and at any other location of interest in the field under test. The inclusion of benchmarks in the adjustment requires the evaluation of the uncertainty matrix associated with the fluences in the benchmark experiments in addition to the evaluation of the uncertainty matrix associated with the field under test, and the cross-uncertainty matrices for the correlated quantities. Unfortunately, applications [3] of the methodology have been few and the original code package has not been maintained.

New GLLS Code

The GLLS methodology was introduced to reactor physics, in particular to fast reactor physics, approximately 40 years ago [4,5]. The sensitivity/uncertainty (S/U) techniques, based on the GLLS methodology, were further developed in the 1970s and 1980s for a variety of applications, including nuclear data evaluation [6], fast reactor design studies [7], and reactor pressure vessel damage predictions [3]. Recently

Manuscript received June 20, 2005; accepted for publication April 19, 2006; published online June 2006. Presented at ASTM Symposium on Reactor Dosimetry, 12th International Symposium on 8–13 May 2005 in Gatlinburg, TN; D. W. Vehar, D. M. Gilliam, and J. M. Adams, Guest Editors.
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a similar methodology has been applied to criticality safety analysis, and a GLLS code has been developed within the SCALE code system [8] to determine biases and uncertainties in neutron multiplication factors by consolidating differential data and benchmark integral experiments. The adjustment code uses the GLLS method to consolidate a prior set of integral responses measured in critical benchmark experiments and a corresponding set of calculated values obtained using the SCALE code system. The code improves the initial estimates for calculated and measured responses by varying the nuclear data used in the transport calculations as well as the values of the measurements, taking into account their correlated uncertainties, in the sense that the most self-consistent set of data is obtained. This approach forces the modified estimates of the calculated and measured responses to agree, while at the same time constraining the data variations to minimize a generalized chi-square. This ensures maximum overall consistency in the set of calculated and measured responses for a specified set of data and experimental uncertainties; thus, the posterior results represent the "best estimates" for the true response values. Consolidation of the original integral experiment data and calculated results reduces the prior uncertainty in the response estimates, since additional information has been incorporated, compared with either the measured or calculated results alone.

This paper describes the TSURFER code (tool for sensitivity/uncertainty analysis of response functionals using experimental results), which is a functional module in the SCALE S/U analysis methodology [8]. The main functions of the code are (a) to compute uncertainties in calculated integral responses, such as k_{eff}, due to uncertainties in the input nuclear data, and (b) to analyze measured responses from benchmark integral experiments in order to establish the bias and associated uncertainty in some application response that has been calculated. As a result, the observed discrepancies between the measured and calculated responses are reduced, as well as the uncertainties associated with the adjusted quantities.

The SCALE nuclear analysis system is comprised of (a) calculation modules (codes) and (b) control modules (sequences) that execute one or more codes to perform a particular function. Other modules in SCALE perform complementary S/U calculations and prepare input files for the TSURFER code. Some other routines involved with S/U are summarized below. Puff-III is described in Ref. [9], and descriptions of the other routines can be found in the SCALE 5 documentation [8]. The TSURFER code represents a component within the overall S/U capability of the SCALE system.

TSURFER provides an alternative approach to the traditional trending analysis used by the criticality safety community to determine "computational biases." Traditional trending analyses estimate the computational bias based on observed trends between calculated k_{eff} values versus system parameters such as hydrogen-to-fissile ratios (H/X) or energy of average lethargy causing fission (EALF). These physical parameters are widely accepted as reasonable measures of "similarity" between various systems, hence their use as bias predictors. Recent studies have shown that combinations of data sensitivity coefficients, either alone or in combination with cross-section uncertainty information, are also good indicators of system similarity [10]. S/U-based indices can be used in trending analyses similar to the widely used physical parameters. The inputs needed for S/U trending analysis (i.e., calculated and measured responses, sensitivity coefficients, cross-sectional and experimental uncertainties) are almost identical to those needed for GLLS analysis; therefore, it is not surprising that some by-products of TSURFER calculations (similarity coefficients, bias variation versus benchmark experiments) are similar to parameters applied for trending results. However, the TSURFER code can be used to address several other important validation issues.

Not only can the computational bias and the uncertainty be calculated by TSURFER for a given application, but the cumulative "combination" of experimental data from several critical benchmarks can also be used to determine the convergence of the procedure. Questions that can be addressed include the following: How many experiments are needed to verify an application? What degree of correlation between the experiment and the application is necessary to validate the application area? The GLLS methodology has been used to answer these questions [10]. Additionally, this tool is expected to be of value for criticality safety validation even when there are very few or no existing experiments considered to be similar to a particular application area. The GLLS technique is useful under these circumstances since individual experiments can be included that separately validate portions of the application area, even though none can be considered entirely similar [11].

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Types of Responses

A "response" corresponds to a particular integral response *type* (e.g., k_{eff}, reaction rate ratio, material worth, radiation dose) in a particular *nuclear system* (e.g., a benchmark experiment, a power reactor, or a proposed storage arrangement of reactor fuel assemblies). In the TSURFER input, responses may be classified as "*experiments,*" "*applications,*" or "*omitted*."

An *experiment* response has both calculated and measured values input to TSURFER, and these play an active role in the GLLS procedure that attempts to minimize differences between the two results. A value for the uncertainty in the measured response, as well as any response correlations, is also input for experimental responses. Examples of experimental integral responses are the multiplication factor for the GODIVA critical benchmark experiment, the measured ρ^{28} (ratio of epithermal to thermal capture rate for ^{238}U) in the TRX-1 critical benchmark lattice, the coolant voiding reactivity in a pressurized-water reactor (PWR), or a surveillance dosimetry measurement in a PWR.

Applications are responses for which a calculated value is known but no measured value is available. Applications often correspond to hypothetical systems being considered within the context of a design study or a criticality safety analysis for which the computational bias and uncertainty values are desired. Examples of application responses are the multiplication factor (subcritical) for a proposed fuel assembly storage rack or for a shipping cask or the flux at any desired location in a PWR pressure vessel. An application response plays a passive role in the GLLS procedure. Since the application has no experimental values, it does not impact the values of the active responses included in the consolidation procedure. However, conversely, the GLLS procedure may modify the calculated value of the application if it is "similar" to some of the experimental responses. In this case, the application response shares similar data sensitivity characteristics with one or more of the active responses and hence will be indirectly affected by the same data variations that impact the similar experimental responses. This provides a systematic, well-defined method for utilizing experimental benchmark measurements to establish a bias and uncertainty in the calculation of application response or to estimate the fluence and its uncertainty at the quarter-thickness position of a PWR pressure vessel.

A response designated as *omitted* in the TSURFER input neither affects other responses nor is affected by them. These responses are completely isolated from the GLSS procedure. This capability is sometimes useful to easily "turn off" an active system to observe its impact on the application results or on the consistency (chi-square) of the set of remaining experimental responses.

Uncertainties

Experimental Uncertainty

Even "clean" critical benchmark experiments have uncertainties in the nominal system parameters, such as fuel enrichment, impurities, densities, critical dimensions, and numerous other components, that contribute to the observed discrepancy in the measured and calculated responses for the system. In TSURFER the impact of these uncertainties is designated as the "experimental uncertainty" in the response, since this uncertainty will be present even if no simplifications or approximations are made in the model used for the transport computation. The terminology is sometimes a source of confusion. For example, the measured k_{eff} in a critical experiment is usually known to be unity with a very small uncertainty associated with the long, but finite, stable period. While there is little doubt about the value of k_{eff} for a critical experiment, there may be considerable uncertainty in the system parameter values that describe the benchmark configuration. This contribution to the modeling uncertainty could be justifiably considered either "experimental" (because system parameters such as material compositions and dimensions are specified by the experimentalists) or "computational" (because uncertainties in the system parameters affect the calculation model). However, in TSURFER they are designated as experimental uncertainties. In any case, the uncertainty in each system parameter must be propagated to an uncertainty in the measured response. For a k_{eff} response, this may be done experimentally by physically varying the system parameter and measuring the reactivity effect or, more commonly, by performing auxiliary transport calculations to determine the k_{eff} eigenvalue sensitivity.

The response uncertainty components associated with the respective modeling uncertainties in system parameters determine the overall experimental uncertainty. Many benchmark experiment descriptions in

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the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* [12] include information about uncertainties in the system parameters and their estimated impact on the multiplication factor. The benchmark evaluators assign the standard deviations in k_{eff} due to uncertainties in various system parameters based on published or archived experiment descriptions, and sometimes on other considerations [13].

A complication in specifying the experimental uncertainty is how to treat correlations among the different experiments. Response correlations in two benchmark experiments may be caused by factors such as use of the same fuel pins or solutions, the same cladding material and container tank, and common instrumentation (same detectors, hydrometers, etc.). For example, if two different critical experiments use the same fuel material, then it is not justified in the GLLS analysis to conclude that the enrichment in one is too high while the other is too low, even if both differences fall within the specified standard deviation. Our experience and the experience of others [14] have shown that these correlations may not be negligible when applying the GLLS technique to a set of benchmark experiments. Unfortunately, only a limited amount of experiment correlation data has been published, although more is expected to be included in future revisions to the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*. The TSURFER code allows experimental uncertainties caused by uncertainties in system modeling parameters to be input for individual components, and correlation coefficients can be specified for the shared system parameters of each response. This approach provides the capability for users to more easily describe the sources of benchmark experiment correlations, without having to know the overall correlation between two different experiments.

Parameter (Cross-Sectional) Uncertainties

In many instances, the major source of uncertainty in the calculated response is due to uncertainties in basic nuclear data such as microscopic cross sections, fission spectra, neutron yield (nu-bar), and scattering distributions. In dealing with multigroup cross-sectional libraries such as those utilized in typical SCALE calculations, uncertainties due to resonance self-shielding should also be included [15]. The nuclear data uncertainties are described by multigroup covariance matrices that contain variances in individual group cross sections for a given nuclide and reaction type, as well as covariances arising from the correlations between energy groups, and possibly between reactions and materials. Correlations, as well as uncertainties in nuclear data, can have a significant impact on the overall uncertainty in the calculated response; thus, it is important to include these in the TSURFER calculations.

Beginning with VERSION V formats, ENDF/B evaluations have had the capability to include covariance information describing uncertainties in the basic nuclear data [16]. ENDF/B-V included covariance data for several important materials needed in criticality safety and nuclear reactor calculations, but many materials had no covariance data in VERSION V. When ENDF/B-VI was released in 1989, it contained significant revisions to many of the cross-section evaluations in ENDF/B-V. For example, a more rigorous resonance treatment based on the Reich-Moore formalism was used to represent the cross sections of most nuclides. However, new covariance data were not evaluated in many cases, and, in fact, several evaluations that previously had covariance data in ENDF/B-V do not have corresponding data in VERSION VI. Notable among these are H, ^{10}B, N, O, and ^{239}Pu. Thus the ENDF/B covariance data are still incomplete at this time.

TSURFER calculations typically utilize the nuclear data covariance libraries distributed with the SCALE code package. Like the SCALE cross-sectional libraries, the covariance libraries currently available for S/U analyses were generated from ENDF/B-V evaluations. Because several important nuclides do not have uncertainty data in ENDF/B-V, approximate covariance evaluations produced by Argonne National Laboratory (ANL) for 30 additional materials [17] were obtained to supplement the ENDF data. Furthermore, fission spectrum uncertainties are not normally tabulated in the ENDF/B evaluations but can be important contributors to the overall uncertainty for some applications. Therefore, uncertainty information for the fission spectra of ^{235}U, ^{239}Pu, and ^{252}Cf was also added to the files. The generation of the fission spectrum uncertainties is described in Ref. [18].

Evaluated covariance files represent cross-sectional uncertainties using ENDF/B formats such as absolute or fractional variance components defined over fixed energy intervals, fractional variance components correlated over all energy intervals, and fractional variance components correlated over arbitrary energy intervals. The basic evaluated uncertainty files were processed by the PUFF-III computer code [9] into multigroup covariance data in the SCALE 44-neutron group structure. Two multigroup covariance libraries

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TABLE 1—*Nuclides contained in 44GROUPV5COV library.*

Identifier	Isotope	Identifier	Isotope
13 027	Al-27	11 023	Na-23
95 241	Am-241	28 000	Ni
79 197	Au-197	92 237	Np-237
5010	B-10	8016	O-16
6012	C-12	82 000	Pb
27 059	Co-59	94 239	Pu-239
24 000	Cr	94 240	Pu-240
9019	F-19	94 241	Pu-241
26 000	Fe	94 242	Pu-242
1001	H-1	14 000	Si
49 115	In-115	90 232	Th-232
3006	Li-6	92 235	U-235
3007	Li-7	92 238	U-238
25 055	Mn-55	98 252	Cf-252
7014	N-14		

are currently available in the SCALE code package. The library named 44GROUPV5COV contains covariance matrices for all materials that have relative covariance information given in ENDF/B-V (Table 1). The other library, named 44GROUPANLCOV, contains the ENDF/B-V uncertainty information, plus relative covariance matrices for the additional nuclides processed from the ANL evaluations.

The covariance file should include standard deviations as well as correlations in the cross sections for different energy groups, reaction types, and materials used in the response calculations. Ideally, the covariance file should contain data for all materials, reactions, and energy groups that impact the set of responses considered in the GLLS analysis; however, covariance data are not currently available for some materials in the SCALE nuclear data libraries. For these data the user may input a default relative standard deviation and a default correlation coefficient that are used to define the uncertainty matrix of any nuclide-reaction combination that has no data in the covariance file. The default uncertainty value defines the variance in the group cross sections, which lies along the diagonal of the covariance matrix. TSURFER assumes that neighboring groups are correlated and assigns the input correlation coefficient to the matrix elements immediately to the left and right of the diagonal. All other elements in the multigroup covariance matrices are set to zero, indicating no "long-range" correlation among the groups. Values for the default relative standard deviation and neighboring correlation coefficient are set by TSURFER input parameters. These are used to define uncertainties for data that have no covariance information on the input file and that have sensitivities greater than a threshold value also specified as an input parameter. All these input parameters have standard default values.

Sensitivities

All active and passive responses considered in the GLLS analysis should have sensitivity data provided for each material and reaction type that significantly impact the response. The sensitivity coefficients are precalculated using other SCALE modules and are stored in individual files for each response included in the TSURFER analysis. The locations of the sensitivity files are specified in the TSURFER input data so that they can be read during the calculation. It is not required that all of the input sensitivity files have the same group structures; for example, the sensitivity coefficients for one response may have been computed using a 238-group cross-sectional library, while sensitivities for another response could have a 44-group structure. Whatever the group structure of the sensitivity data, it will be mapped into the same group structure as the covariance file. At present, the covariance files in SCALE use the standard 44-group structure.

Consistency

The value of *chi-square* χ^2 is a key to the proper interpretation of the TSURFER results. The χ^2 statistic is a measure of the overall consistency of the set of experimental values of the benchmark responses and the nuclear parameters used for their calculation. TSURFER edits the total χ^2 value, as well as individual values

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TABLE 2—*HST systems properties.*

System no.	Name	c	Indep. χ^2	Diag. of χ^2
1	hst009-01	1.0033E+00	0.0646	1.1857
2	hst009-02	1.0038E+00	0.0972	2.6007
3	hst009-03	1.0029E+00	0.0681	2.4198
4	hst009-04	9.9681E−01	0.0937	1.7902
5	hst010-01	1.0030E+00	0.0965	17.3072
6	hst010-02	1.0038E+00	0.1527	**27.4728**
7	hst010-03	1.0004E+00	0.0013	0.2446
8	hst010-04	9.9859E−01	0.0205	3.7139
9	hst011-01	1.0067E+00	0.5041	**37.0796**
10	hst011-02	1.0025E+00	0.0699	5.0769
11	hst012-01	1.0019E+00	0.0567	1.6014
12	hst013-01	9.9980E−01	0.0265	0.399
13	hst043-01	9.9752E−01	0.0104	0.3155
14	hst043-02	1.0078E+00	0.8847	**20.6383**
15	hst043-03	1.0028E+00	0.1981	3.3844
16	hst042-05	1.0000E+00	0	0
17	hst042-06	1.0003E+00	0.0011	0.0105
18	hst042-07	1.0011E+00	0.016	0.1778
19	hst042-08	1.0014E+00	0.0265	0.3112

for each experiment. The individual χ^2 values may suggest which experiments contain inconsistencies (i.e., the magnitude of the measured-to-calculated k_{eff} discrepancy is larger than their combined uncertainties). However, the source of inconsistencies may well lie in the nuclear input parameters and, although all responses have small individual χ^2 values, the whole suite may not prove to be consistent. Values of chi-square per degree of freedom (χ^2/n) usually should be within about 20 % of unity for defensible results. Results in which this test is not met may still be valid. However, in general, these results should be viewed with skepticism unless the reasons for the test failure are understood.

Several established methods can be used to modify the value of χ^2/n. One includes a reevaluation of experimental uncertainties and their correlations. A high value of χ^2 indicates that the predicted data variations are well outside the bounds of the standard deviations. If the input experimental uncertainties are underestimated, the data movements can be too extreme and are reflected in high χ^2 values. Values of χ^2 that are too low often suggest that the input experimental uncertainty estimates might be too high, and again a reevaluation should be performed. Thus, it is quite important to utilize *realistic* (not "conservative") estimates for the uncertainties in nuclear data and experimental measurements. Yeivin et al. [19] presented a detailed discussion of inconsistencies and demonstrated a technique for rejecting the responses most responsible for the inconsistencies of the whole suite. An alternative rejection technique based on the value of the "diagonal contribution to χ^2," which is the product of the square of the deviation of the measured from the calculated response values and the respective diagonal value of the inverse of the deviation uncertainty matrix, is presented here.

Twenty-two International Criticality Safety Benchmark Evaluation Project (ICSBEP) [12] highly enriched thermal solution (HST) systems were used for this analysis. Throughout the calculations of proposed adjustments the last three responses (20, 21, and 22) were used only as "applications;" that is, they only passively participated in the adjustment. The chi-square per degree of freedom χ^2/n of this setup was 4.2598, an unacceptable result. The ICSBEP names, calculated k_{eff}, and the χ^2 properties for each of the remaining 19 systems are presented (Table 2). System 9 has the highest value of the "diagonal contribution to χ^2" and was thus excluded from the adjustment campaign, resulting in a χ^2/n of 3.4763, which is still too high. Next, system 6 was excluded and χ^2/n was reduced to 1.6267. Next, system 14 was deactivated. The adjustment campaign, without systems 9, 6, and 14, now yielded a χ^2/n value of 0.9976, which is quite acceptable. One could have guessed a priori that these three systems are candidates for rejection due to the deviation of their calculated k_{eff} values from the experimental value of 1. However, their individual χ^2 values do not deviate from unity and the criterion we chose takes into account the global effect of the information analyzed. The k_{eff} values of each of the systems are depicted in Fig. 1 for each of the adjustment campaigns. The curve labeled "c" shows the original calculated k_{eff} values; "a-4.3," the adjusted k_{eff} values using all 19 systems; "a-3.5," the adjusted k_{eff} values after system 9 was rejected; and

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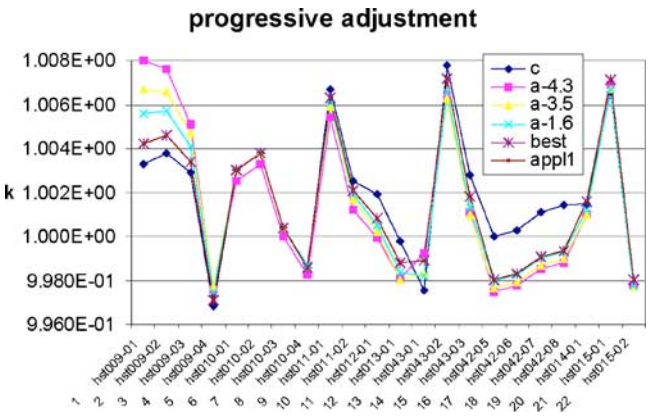

FIG. 1—*Inconsistent systems rejection. (appll is not visible since it is the same as best).*

"a-1.6," the adjusted values after the rejection of systems 9 and 6. The curve labeled "best" indicates the adjusted k_{eff} values after the rejection of the three systems 9, 6, and 14, resulting in a χ^2/n of ~ 1.

It is interesting to note that although there are systems that seem insensitive to the consistency parameter, the adjusted k_{eff} values of systems 3, 2, and 1 are very sensitive to the inclusion of inconsistent systems. The effect is most profound in system 1, HST009-01. The curve labeled "appl1" is the result of an adjustment in which system 1 was also used as an application. There is no difference between the "best" and "appl1" curves, indicating the success of the method. Although system 1 did not actively participate in the adjustment, its adjusted value is the same as its value when actively participating in the adjustment. The adjusted values of system 1, without inactivating the inconsistent systems, differ by a few "mille-k" from the "best" value. The adjusted k_{eff} value of system 1 without the exclusion of any inconsistent system differs from both the experimental and calculated values by more than its experimental uncertainty (4 mille-k).

Summary and Conclusions

TSURFER, a GLLS module of SCALE, and its features were described followed by a numerical illustration showing the importance of rejecting inconsistent systems.

Acknowledgments

This work was sponsored by the U.S. Department of Energy under the Applicable Ranges of Bounding Curves and Data (AROBCAD) element of the Nuclear Criticality Safety Program (NCSP).

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