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Abstract

This paper documents the results obtained in an adjustment study of cross section parameters as well as k_{eff} responses of 19 spherical plutonium critical assemblies, utilizing the new TSURFER (Tool for Sensitivity/Uncertainty Analysis of Response Functionals Using Experimental Results) module. Special attention was devoted to the sensitivity of the results to the available variance-covariance data and supplements for the responses and parameters.

KEYWORDS: Adjustment, variance-covariance matrices, uncertainties, plutonium critical assemblies

1. Introduction

The Generalized Linear Least Squares Methodology (GLLSM) is implemented in the TSURFER (Tool for Sensitivity/Uncertainty Analysis of Response Functionals Using Experimental Results) module of the internal development version of the SCALE 5.1 system [1]. The methodology utilizes the measured values of **responses, *r*,** such as k_{eff}, and reaction rates, as well as their respective uncertainties, given as a variance-covariance matrix, C_r. Also used is a series of **parameters, *p*,** such as cross sections, number of neutrons emitted in fission, and fission spectra, as well as their respective uncertainties, given as a variance-covariance matrix, C_p. Both the responses and the parameters are represented as vectors of different dimensions corresponding to the respective number of responses and the number of parameters, and the uncertainties are square matrices of corresponding dimensions. The methodology combines the information and results in the reduction of the uncertainties of both responses and parameters. These modified parameters, having a smaller uncertainty, are used in turn, for example, to predict k_{eff} values in criticality safety applications and provide an estimate for the bias in the computations.

The modified parameter and response values [2] are

$$p' = p - C_p S^{\dagger} C_d^{-1} d \ , \quad r' = r + C_r C_d^{-1} d \ , \tag{1}$$

where $d = \bar{r}(p) - r$ is the deviation vector of the calculated response values from their respective measured values. The matrices denoted by C are the respective variance-covariance matrices or "uncertainties," where

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$$C_d = C_{\bar{r}} + C_r - C_{\bar{r}r} - C_{r\bar{r}} = S\,C_p S^\dagger + C_r - S\,C_{pr} - C_{rp} S^\dagger \quad . \tag{2}$$

The matrices S are the sensitivities of the responses to the parameters, while the matrix C_{rp} and its transpose C_{pr} represent possible parameter-response correlations. Usually such a priori correlations are not present in reality and can be omitted.

The new uncertainties in the modified (i.e., adjusted) parameters and in the adjusted responses and the resulting new correlations (this time also between adjusted parameters and adjusted responses) are given by

$$C_{p'} = C_p - C_p S^\dagger C_d^{-1} S C_p,\; C_{r'} = C_r - C_r C_d^{-1} C_r,\; C_{p'r'} = C_p S^\dagger C_d^{-1} C_r \quad . \tag{3}$$

Since the uncertainty matrices are, by their definition as variance-covariance matrices, positive definite, the uncertainties are reduced in such a campaign. The consistency of all data used is given by chi square, which in our case reduces to the simple form of $\chi^2 = d^\dagger C_d^{-1} d$.

The work described here is the analysis of the dependency of the adjustment results on various features and assumptions in such a process utilizing the TSURFER module. The analysis involves 19 benchmark metallic spherical plutonium cores, bare and reflected. In particular, the sensitivity of the results to the procedures used to supplement missing parameter uncertainties, as well as to the representation of the response uncertainty correlations was checked.

2. Plutonium Assemblies

The data of the 19 metallic plutonium assemblies are from the International Handbook of Evaluated Criticality Safety Benchmark Experiments [3]. A short description of the assemblies utilized in our analysis and their ICSBEP names are given in Table 1. The assemblies are not arranged in Table 1 as in the handbook but rather according to similarity, (i.e., bare systems), then natural uranium-reflected systems and then other reflected systems.

Table 1: Overview of the metallic plutonium systems.

System I.D.	ICSBEP I.D.	Benchmark Title
1	pmf-001	Jezebel (δ, 4.5 at.% 240Pu) US bare Pu sphere
2	pmf-002	Jezebel (δ, 20.1 at.% 240Pu) US bare Pu sphere
3	pmf-022	Bare (δ, 98% 239) VNIIEF layered Pu sphere
4	pmf-029	Bare (α, 88% 239) VNIIEF layered Pu sphere
5	pmf-010	(δ, 4.9 at.% 240Pu) US (Planet) Pu sphere, 1.625 in. U reflected
6	pmf-006	Flattop (δ, 4.8 at.% 240Pu) US Pu sphere, 19.6088 cm U reflected
7	pmf-008	(δ, 5.1 wt.% 240Pu) US (Thor) Pu sphere, 24.57 cm thorium reflected
8	pmf-005	(δ, 4.9 at.% 240Pu) US (Planet) Pu sphere, 4.699 cm tungsten alloy reflected
9	pmf-018	(δ, 4.9 at.% 240Pu) US (Planet) Pu sphere, 1.452 in. Be reflected
10	pmf-030	(α, 88% 239) VNIIEF layered Pu core, 4.49 cm graphite reflected
11	pmf-023	(δ, 98% 239) VNIIEF layered Pu core, 2.35 cm graphite reflected
12	pmf-027	(δ, 89% 239) VNIIEF layered Pu core, 5.58 cm polyethylene reflected
13	pmf-024	(δ, 98% 239) VNIIEF layered Pu core, 1.55 cm polyethylene reflected
14	pmf-031	(α, 88% 239) VNIIEF layered Pu core, 3.69 cm polyethylene reflected
15	pmf-011	(α, 5.18 at.% 240Pu) US Pu sphere, 10 in. water reflected
16	pmf-025	(δ, 98% 239) VNIIEF layered Pu core, 1.55 cm steel reflected
17	pmf-026	(δ, 98% 239) VNIIEF layered Pu core, 11.9 cm steel reflected
18	pmf-028	(δ, 89% 239) VNIIEF layered Pu core, 19.65 cm steel reflected
19	pmf-032	(α, 88% 239) VNIIEF layered Pu core, 4.49 cm steel reflected

3. Response Experimental Uncertainty and Correlations

Even "clean" critical benchmark experiments have uncertainties in the nominal system characteristics, such as fuel composition and enrichment, impurities, densities, critical dimensions, and other components, that contribute to the observed discrepancy in the measured and calculated responses for the system. 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 inferred k_{eff} from measurements of 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 characteristic values that describe the benchmark configuration.

This contribution to the modeling uncertainty could be justifiably considered either "experimental" (because system characteristics such as material compositions and dimensions are specified by the experimentalists) or "computational" (because uncertainties in the system characteristics affect the calculation model). However, in TSURFER they are designated as experimental uncertainties. In any case, the uncertainty in each of the system characteristics 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 characteristics 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 characteristics determine the overall experimental uncertainty. Many benchmark experiment descriptions in the International Handbook of Evaluated Criticality Safety Benchmark Experiments [3] include information about uncertainties in the system characteristics and their estimated impact on the multiplication factor. The benchmark evaluators assign the standard deviations in k_{eff} due to uncertainties in various system characteristics based on published or archived experiment descriptions, and sometimes on other considerations [4].

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 shells and common instrumentation (same detectors, analysis methods, etc.). For example, if two different critical experiments use the same fuel shells, then it is not justified in the GLLSM 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. 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 characteristics to be input for individual components, and correlation coefficients can be specified for the shared system characteristics 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.

As can be seen in Table 1 the plutonium cores are of varying composition (% of ^{239}Pu) and of different metallic phase (α, δ) (i.e., densities). Special attention was paid in order to identify cores that have the same composition, shells, phase and assembly machine, thus being highly correlated. In our analysis the various uncertainty sources in k_{eff} of the different cores were adopted from the handbook when available. The TSURFER capability to generate a covariance matrix of the responses based on its input, which consists of common uncertainty sources and of the assumed correlation between the contributions of the same uncertainty source for different assemblies, was utilized.

The systems 4, 10, 14, and 19, for instance, use the same assembly machine at the same laboratory; have the same core shells, (i.e., same dimensions for most core shells, same composition, impurities and density) and use the same experimental and analytical procedures. The first one is a bare sphere, and the others have graphite, polyethylene and steel reflectors, respectively. Correlations of 0.95, 0.85, 0.5 and 0.0, in turn, were assumed

for all common source uncertainty contributions k_{eff}. Systems 3, 11, 13, 16 and 17 are similarly correlated and were treated accordingly.

4. Parameter Uncertainty Information

The parameter uncertainty information is obtained by the TSURFER module from a file the name of which is specified in the input data. The locations of the sensitivity files, pregenerated by other SCALE modules, are also specified in the TSURFER input data so that they can be read during the calculation when needed. These files contain the sensitivities of the requested response, k_{eff} for instance, to each and every reaction cross section for every material (isotope) in the system description.

Our analysis used the parameter uncertainty covariance files generated by PUFF-III [5] from ENDF/B-V and denoted in SCALE 5 as 44GROUPANLCOV. The TSURFER module looks for the uncertainty files needed according to the sensitivities of each response. When the sensitivity is greater than a given threshold value, 0.001 in our case, and there is no variance-covariance matrix available in the parameter uncertainty file, TSURFER generates its own covariance matrix with a given uniform **D**efault relative **S**tandard **D**eviation, DSD, and a **D**efault **CO**rrelation for adjacent groups, DCO. The parameter uncertainty file used in this work does not have covariance matrices for quite a few nuclide-reaction pairs. For instance, the file is missing elastic scattering covariance matrices for various plutonium isotopes and for carbon, as well as fission spectrum covariance matrices for the higher plutonium isotopes. Because the fission spectra, being normalized to one, have strong anti-correlations and the elastic scattering may have a positive correlation with neighboring energy groups, the DCO parameter was set to zero (i.e., no correlations). The sensitivity of TSURFER results to the DSD value was tested and is depicted in Figs. 1 and 2. The DSD values of 10, 5, and 0% (i.e., the relative standard deviations of the cross sections or the fission spectra are 10, 5, or 0%) vary the adjusted k_{eff} values only slightly. In Fig. 1, the adjusted k_{eff} values for all 19 systems are given for the 3 DSD values. Because a few systems with high k_{eff} values that deviate significantly from unity had to be rejected from our analysis, as will be explained later, Fig. 2 zooms in on the adjusted k_{eff} values for the first 15 systems. It was decided that a DSD value of 5% will be used for the rest of the analysis because this value is still reasonable for fission spectra and also for the elastic scattering, and because the results do not deviate by much from the 0% case.

5. 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 for each experiment. The individual χ^2 values (i.e., $\chi^2_{ind} = d_i[(C_d)_{ii}]^{-1} d_i$) 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.

Since all the responses and parameters and their respective uncertainties were not consistent, as evaluated with the $\chi^2 = d^{\dagger} C_d^{-1} d$ statistic, some responses had to be rejected. Yeivin et al. [6] presented a detailed discussion of inconsistencies and demonstrated a technique for rejecting the responses most responsible for the inconsistencies of the whole suite. Starting with all responses, N = 19, the value of χ^2/N is much too high, indicating that some systems have to be rejected. We eliminate one response at a time and evaluate χ^2/n for the remaining systems. The response, the elimination of which leads to the lowest value of χ^2/n for the remaining set, is obviously the least consistent one and is thus excluded from the analysis. The procedure is now applied to the remaining set of 18 systems, and the next system least consistent is rejected. This procedure is repeated again until χ^2/n for the remaining set of systems is equal to or close to unity. This procedure is depicted in Figure 3. The top line indicates that system No. 16 (pmf-025) is least consistent with all other benchmarks and with the parameters, (i.e., cross sections, etc.). Rejecting this system the procedure indicates (next line at χ^2/n=4) that system No. 19 has to be rejected and so on. An alternative and much faster rejection technique [7] is 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, that is, $\chi^2_{dia} = d_i [C_d^{-1}]_{ii} d_i$. The systems with the highest values of the "diagonal contribution to χ^2," are eliminated one at a time until χ^2/n for the remaining set of systems is equal to or close to unity. The TSURFER code has the ability to automatically eliminate experiments with high χ^2 values.

6. Sensitivity to Response Correlations

The rejection of the least consistent assemblies from the campaign resulted in a consistent set of critical assemblies on which the importance of the correlations of the responses was tested. The sensitivity of the adjusted k_{eff} values to the assumed correlations are depicted in Figure 4. It can be seen that there is only a minor difference between the results based on the high values of 0.95 or 0.85 correlations and that there can be a difference of more than 0.1% in the k_{eff} values if no correlations are taken into account. It should be recalled that the experimental uncertainty in the determination of k_{eff} is of the order of 0.1%.

7. Conclusions

An adjustment study of 19 plutonium benchmark critical assemblies indicated that the parameter (cross section) data base and response (k_{eff}) data base are not consistent. The rejection of the least-consistent assemblies from the campaign resulted in a consistent set of critical assemblies on which the importance of the correlations of the responses was tested.

The correlations of the responses should be considered and in the lack of readily available correlations reasonable assumptions should be made based on the experiment description. The results are less sensitive to the exact value of these correlations.

Figure 1: The sensitivity of adjusted (k_{eff}-1) values to DSD.

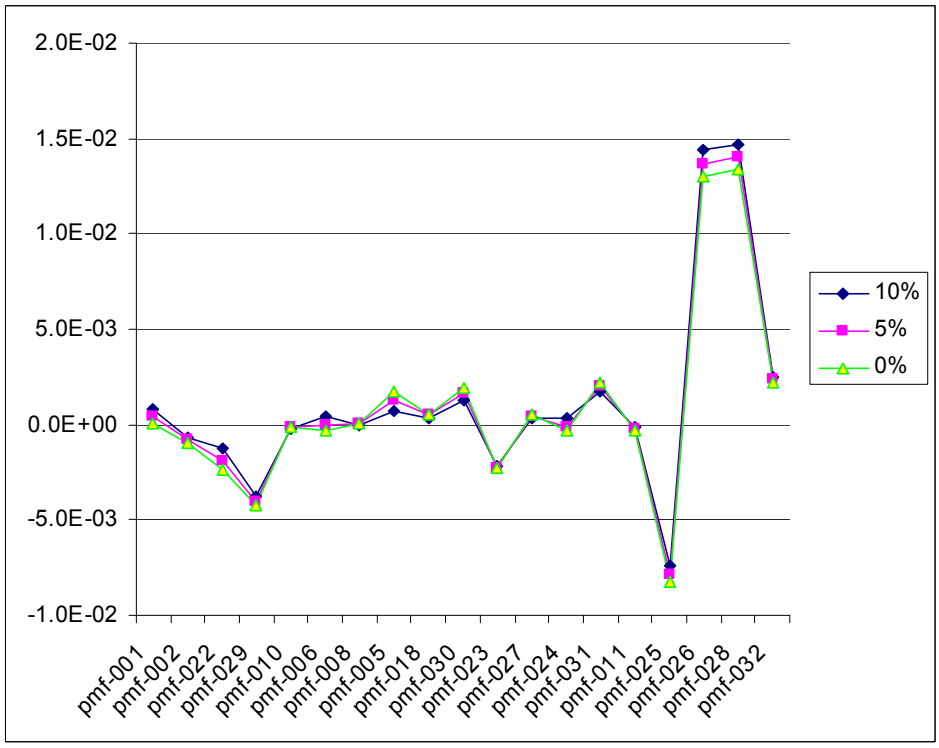


Figure 2: The sensitivity of adjusted (k_{eff}-1) values to DSD (zoom).

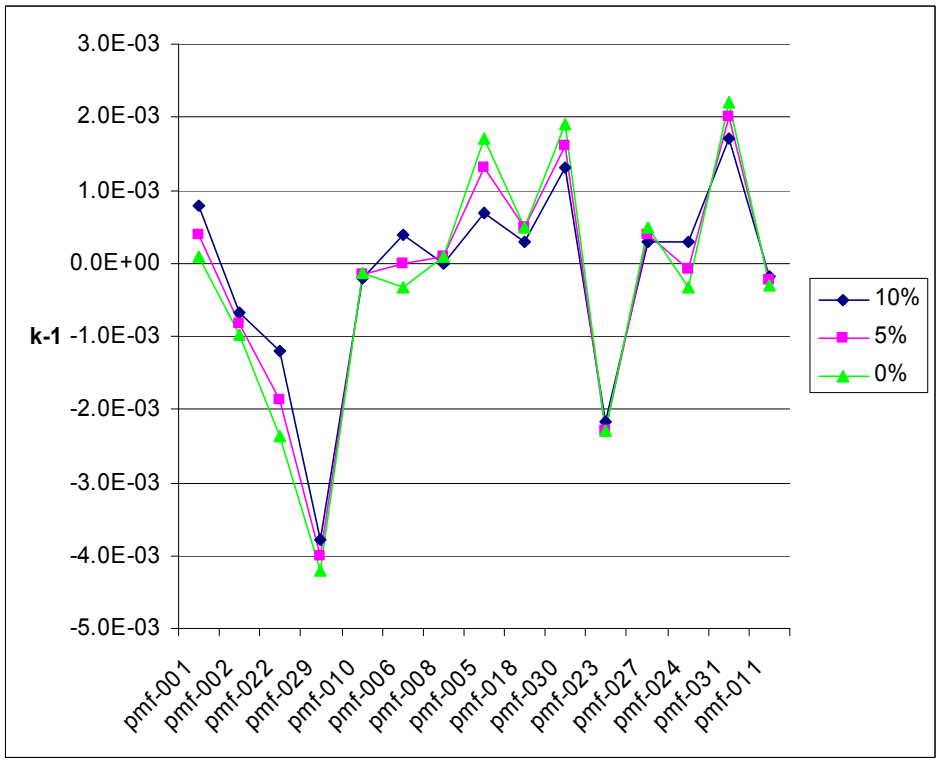


Figure 3: The rejection sequence.

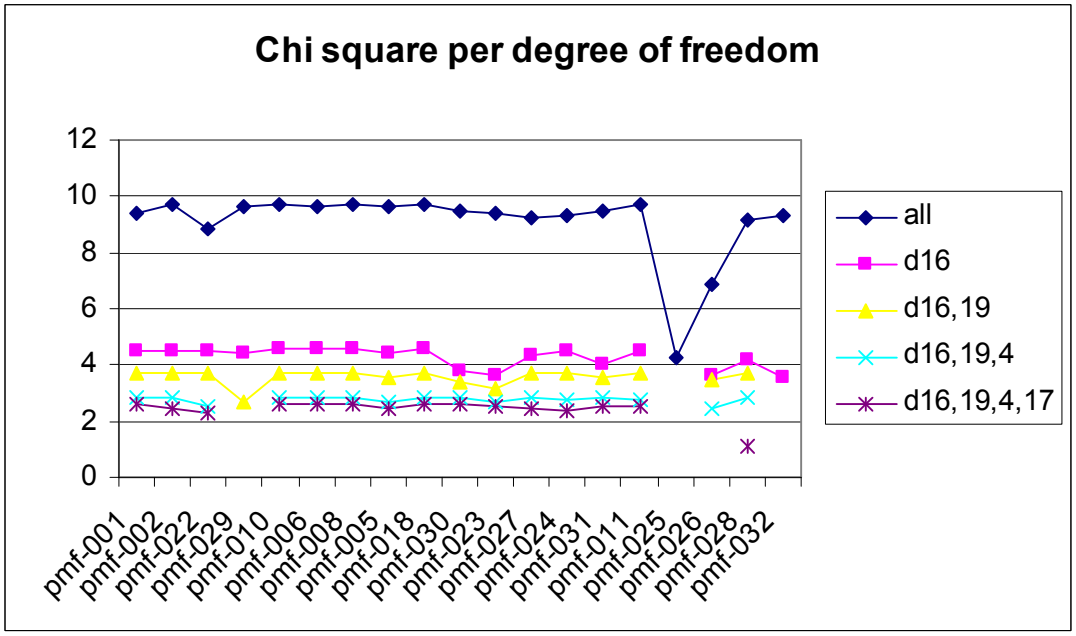
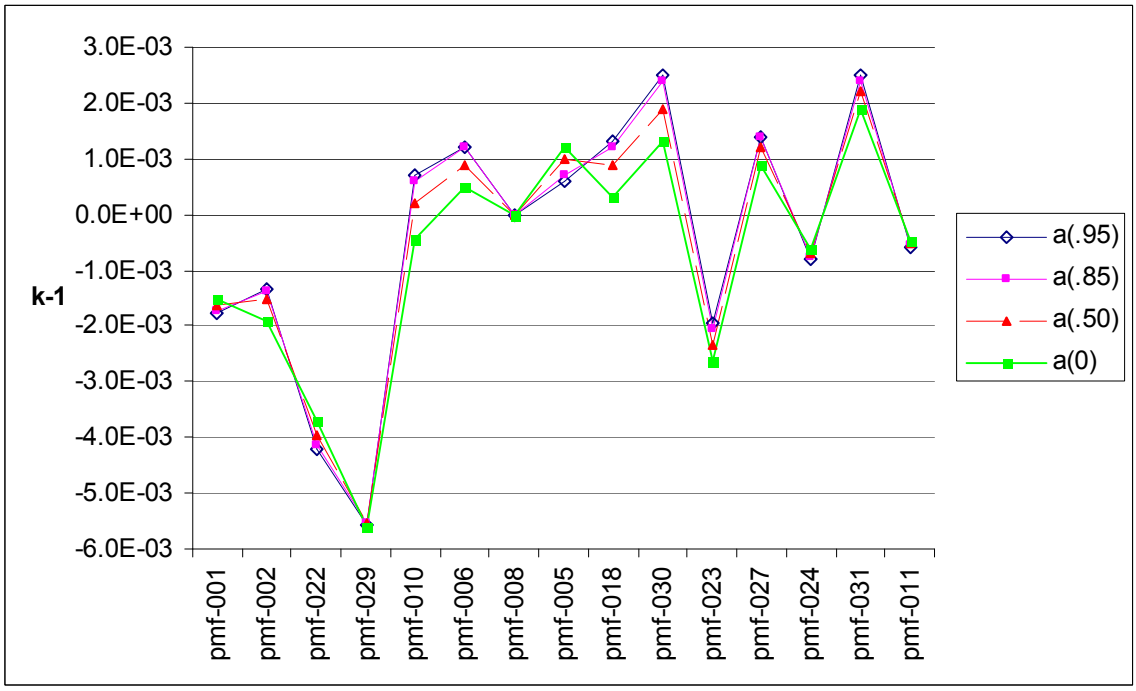


Figure 4: The sensitivity of adjusted k_{eff} values to the assumed correlations.



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