STATISTICAL ANALYSIS OF PST TYPES OF EXPERIMENTS RELATIVE TO EXAMINING "SAFETY APPLICATIONS"

Kirill Raskach*
Obninsk Institute for Physics and Power Engineering
Oak Ridge Associated Universities with U.S. Department of Energy
Oak Ridge National Laboratory Postdoctoral Research Associates Program
Obninsk, Russia

Calvin M. Hopper
Oak Ridge National Laboratory†
P.O. Box 2008, Oak Ridge, TN 37831-6170, USA
Telephone: 865-576-8617
Fax: 865-576-3513
E-mail: hoppercm@ornl.gov

For submission to
ICNC-2007
May 28-June 1, 2007
St. Petersburg, Russia

Notice: This manuscript has been authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes.

*Obninsk Institute for Physics and Power Engineering, Oak Ridge Associated Universities with U.S. Department of Energy ORNL Postdoctoral Research Associates Program.
†Managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725.

STATISTICAL ANALYSIS OF PST TYPES OF EXPERIMENTS RELATIVE TO EXAMINING "SAFETY APPLICATIONS"

Kirill Raskach,[1] Obninsk, Russia

Calvin M. Hopper, Oak Ridge National Laboratory,[2] USA

Introduction

Results of simultaneous analysis of plutonium solution critical experiments reported in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* [1] (IHECSBE) and corresponding conclusions regarding computational accuracy of simple, example safety applications are given in this paper. A suite of those experiments considered in this paper was formed by a research group at the Institute of Physics and Power Engineering (IPPE) for defining experimental uncertainties and correlation coefficients for experimental parameters [2]. In some cases, reevaluated experimental uncertainties and correlation coefficients were provided. That preliminary information was used with the Oak Ridge National Laboratory's prototypic analytic software, TSURFER (***T***ool for ***S***ensitivity/***U***ncertainty analysis of ***R***esponse ***F***unctionals using ***E***xperimental ***R***esults). TSURFER is to be released in SCALE 6, the follow-on to SCALE 5.1[3]. The TSURFER code uses the generalized linear least-squares method to collectively evaluate previously measured integral responses (e.g., k_{eff}) and the corresponding computed values of k_{eff} using the SCALE nuclear analysis code system. TSURFER can vary the nuclear data used in the transport calculations as well as the experimental values themselves, considering correlated uncertainties, to minimize biases between experimental and computed k_{eff} so that the most self-consistent set of nuclear data and experimentally measured values are obtained. Therefore TSURFER provides the opportunity to examine neutron cross-section energy-reaction importance on the bias and uncertainty of calculations as influenced by both neutron-data and critical-experiment correlation coefficients. TSURFER also calculates a similarity parameter, c_k, that characterizes a degree of similarity for two arbitrary (sub-) critical configurations (e.g., between a measured experiment and a safety evaluation computation).

Selection of Reference Benchmarks and Information

The selected experiments, using the benchmark designators from Ref. 1, are provided in Table 1.

The variation in physical parameters of the selected benchmarks ranged as follows:

Hydrogen-to-$^{239+241}$Pu atom ratios: ~ 90 to ~ 2400
Pu density (g Pu/L): ~ 25 to ~ 410
% ^{240}Pu: ~ 2.9 to ~ 23

The SCALE 5.1 ENDF/B-V 238-energy-group neutron cross-section data library and 44-group covariances were used for each of the benchmark computed k_{eff} values, uncertainties, and sensitivities. The experimental uncertainties for the benchmarks were taken from Ref. 1 and the experimental correlation coefficients were taken from Ref. 2. Table 2 provides an example of evaluated uncertainties and their correlations for the PST010 series of benchmarks.

---

[1] Obninsk Institute for Physics and Power Engineering, Oak Ridge Associated Universities with U.S. Department of Energy ORNL Postdoctoral Research Associates Program.
[2] Managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725.

Table 1. Selected critical experiments with plutonium solutions (Ref. 1)

Group	Name	Group	Name	Group	Name
Hanford	PST00201	Valduc	PST01206	PNL	PST00101
	PST00207		PST01207		PST00102
	PST00301		PST01208		PST00103
	PST00305		PST01209		PST00104
	PST00401		PST01210		PST00105
	PST00402		PST01211		PST00106
	PST00403		PST01212		PST00702
	PST00404		PST01213		PST00703
	PST00405		PST01219		PST00705
	PST00406		PST01220		PST00706
	PST00411		PST01221		PST00708
	PST00413	PNL-slabs	PST02403		PST02005
	PST00501		PST02406		PST02007
	PST00507		PST02410		PST02008
	PST00509		PST02416		PST02101
	PST00602		PST02421		PST02102
	PST01001		PST02510		PST02103
	PST01002		PST02517		PST02104
	PST01003		PST02522		PST02105
	PST01004		PST02531		
	PST01008		PST02536		
	PST01009		PST02542		
	PST01010		PST02606		
	PST01011		PST02612		
	PST01014		PST02616		
	PST01101		PST02619		
	PST01105				
	PST01108				
	PST01111				

Table 2. Example evaluated experimental uncertainties and correlations for PST010 benchmarks

	Unc %	PST01001	PST01002	PST01003	PST01004	PST01008	PST01009	PST01010	PST01011	PST01014
PST01001	0.57(0.48)*	1.00								
PST01002	0.57(0.48)	0.42(0.59)	1.00							
PST01003	0.57(0.48)	0.42(0.59)	0.42(0.59)	1.00						
PST01004	0.57(0.48)	0.42(0.59)	0.420.59)	0.55(0.76)	1.00					
PST01008	0.57(0.48)	0.49(0.68)	0.42(0.59)	0.42(0.59)	0.42(0.59)	1.00				
PST01009	0.57(0.48)						1.00			
PST01010	0.57(0.48)			0.06(0.09)	0.06(.09)		0.42(0.59)	1.00		
PST01011	0.57(0.48)						0.42(0.59)	0.48(0.67)	1.00	
PST01014	0.57(0.48)						0.42(0.59)	0.42(0.59)	0.42(0.59)	1.00

* All values in parentheses are those prior to reevaluation.

Definitions of Example Safety Applications

Computational accuracies or biases were determined for simple subcritical (k_{eff} = 0.97) systems that were represented by fully water-reflected, spherical geometry steel tanks filled with plutonium solutions having varied concentrations. Tank diameters were determined for the k_{eff} = 0.97 condition. The materials of consideration, geometry, and computed target k_{eff} are provided in Table 3.

Table 3. Descriptions of safety applications

Reactor-grade plutonium (74 wt % Pu-239, 19 wt % Pu-240, 6 wt % Pu-241, 1 wt % Pu-242)								
Parameter \ Case	**Case-1**	**Case-2**	**Case-3**	**Case-4**	**Case-5**	**Case-6**	**Case-7**	**Case-8**
H/Pu	16.89	29.81	99.54	298.7	597.6	993.4	1495	1991
H/(Pu-239+Pu-241)	21.09	37.23	124.3	373.1	746.5	1241	1867	2487
G_{Pu}, g/L	736.3	622.9	239.6	85.12	43.23	26.17	17.44	13.12
R_{sol}	22.78	18.78	16.57	16.26	17.99	21.38	27.58	38.08
k_{eff}	0.9677	0.9680	0.9678	0.9674	0.9677	0.9681	0.9686	0.9691
Weapon-grade plutonium (95 wt % Pu-239, 4.5 wt % Pu-240, 0.5 wt % Pu-241)								
Parameter \ Case	**Case-1**	**Case-2**	**Case-3**	**Case-4**	**Case-5**	**Case-6**	**Case-7**	**Case-8**
H/Pu	16.89	29.81	99.54	298.7	597.6	993.4	1495	1991
H/(Pu-239+Pu-241)	17.68	31.21	104.2	312.7	625.7	1040	1565	2084
G_{Pu}, g/L	735.4	622.1	239.3	85.02	43.17	26.14	17.42	13.10
R_{sol}	18.75	15.07	13.64	13.86	15.34	17.84	21.85	27.27
k_{eff}	0.9672	0.9672	0.9672	0.9668	0.9673	0.9674	0.9681	0.9685

Benchmark Computational Analysis Results

All of the selected critical experiment benchmarks and defined safety applications were computed with TSUNAMI, thereby providing the neutron energy-group-wise sensitivity and uncertainties in calculated k_{eff} values. The sensitivity data were processed with TSURFER, which provides the total χ^2 value per degree of freedom for the experimental dataset. For the initial set of benchmarks, prior to the reevaluaiton, the χ^2 was 1.47. This relatively large total value indicated that there were some inconsistencies among the experimental and/or computed values used in this analysis. The scatter of the percent differences in the computed minus the experimental critical values are shown in Figure 1. The error bars represent one standard deviation of the combined cross-section, experimental, and computational uncertainties.

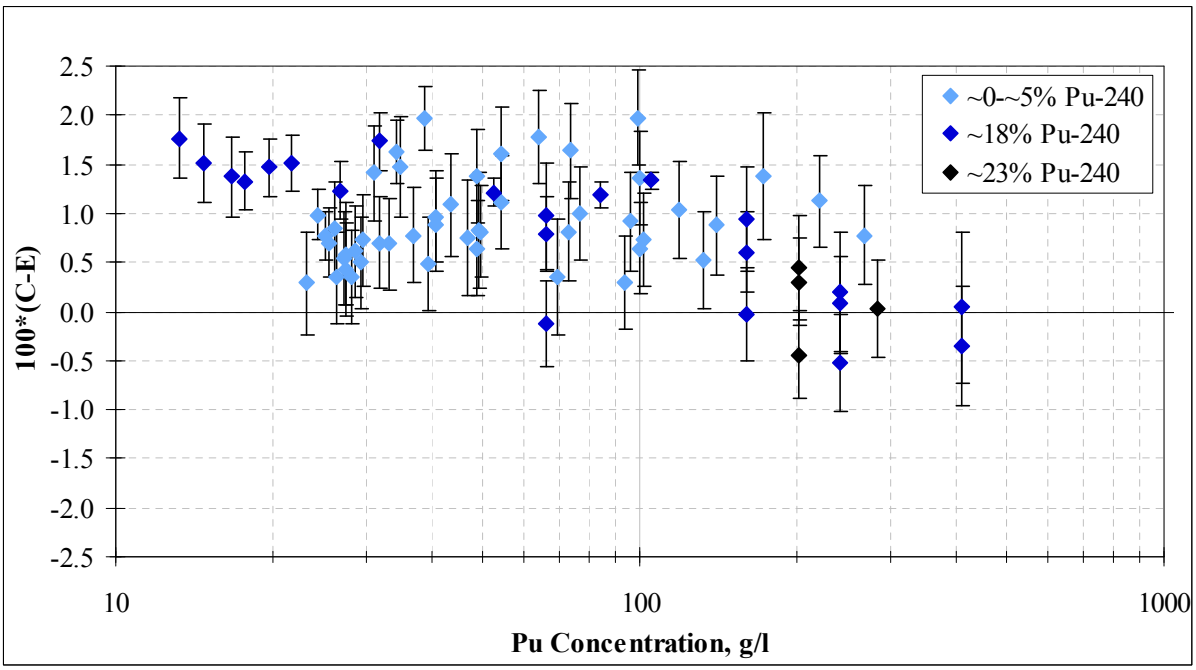

Figure 1. Differences between computed and experimental critical values

The experimental uncertainties and correlation coefficients for a limited set of 33 benchmarks were reevaluated and reconsidered by IPPE. The need for that reevaluation was based upon the similarity correlation coefficient, c_k, within a series of experimental measurements and the chi-square statistic used to test the fit between the computational keff frequency distribution for the benchmark results and the theoretical benchmark frequency distribution. Following reevaluation, the χ^2 value was 0.89.

Graphs of the benchmark data, with experimental standard deviations, and trend plots for the selected safety application predicted biases, with bias prediction uncertainty bands, are provided in Figures 2 and 3 for both reactor-grade (RG) and weapons-grade (WG) plutonium systems. Figure 2 shows the predicted bias and uncertainty band before the reevaluation of benchmark uncertainties and covariances. Figure 3 provides the bias and uncertainty bands after the reevaluation.

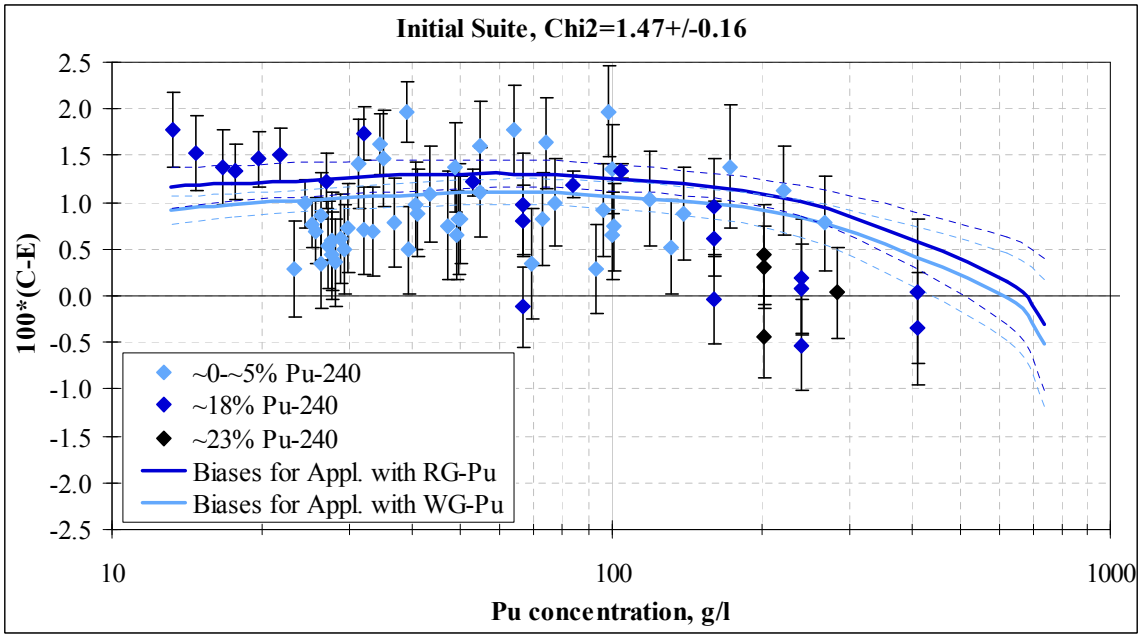

Figure 2. Biases and uncertainty for safety applications before reevaluations

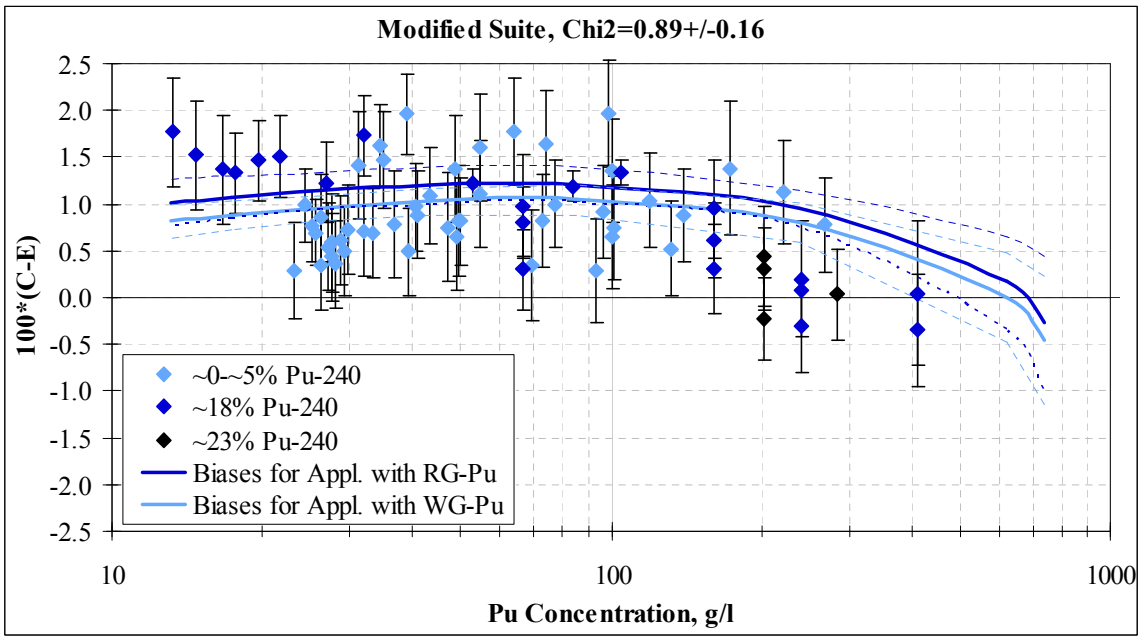

Figure 3. Biases and uncertainty for safety applications after reevaluations

Prior to and after the reevaluation of the benchmark uncertainties and correlation coefficients, the bias and uncertainty for the 16 different safety applications (i.e., 8 weapons grade and 8 reactor grade) were determined with TSURFER. Results of those determinations are provided in Table 4.

Table 4. Computational results for biases and uncertainties prior to and after reevaluations

Plutonium, g/L	Initial dataset				Final dataset			
	Reactor		Weapon		Reactor		Weapon	
	Bias	Bias unc.	Bias	Bias unc.	Bias	Bias unc.	Bias	Bias unc.
735.9	0.31	0.70	0.51	0.68	0.27	0.71	0.46	0.69
622.5	-0.16	0.48	0.01	0.47	-0.16	0.48	-0.01	0.48
239.5	-1.02	0.17	-0.83	0.20	-0.96	0.19	-0.80	0.21
85.07	-1.29	0.15	-1.10	0.14	-1.21	0.18	-1.04	0.16
43.20	-1.29	0.16	-1.09	0.13	-1.20	0.19	-1.02	0.14
26.16	-1.25	0.17	-1.03	0.12	-1.15	0.20	-0.96	0.13
17.43	-1.20	0.19	-0.97	0.13	-1.08	0.22	-0.88	0.15
13.11	-1.16	0.21	-0.91	0.16	-1.02	0.24	-0.82	0.18

The TSURFER computational results before benchmark uncertainty, covariance, and estimated cross-section modification, taking into account cross-section uncertainties and covariances, are presented in Figure 4.

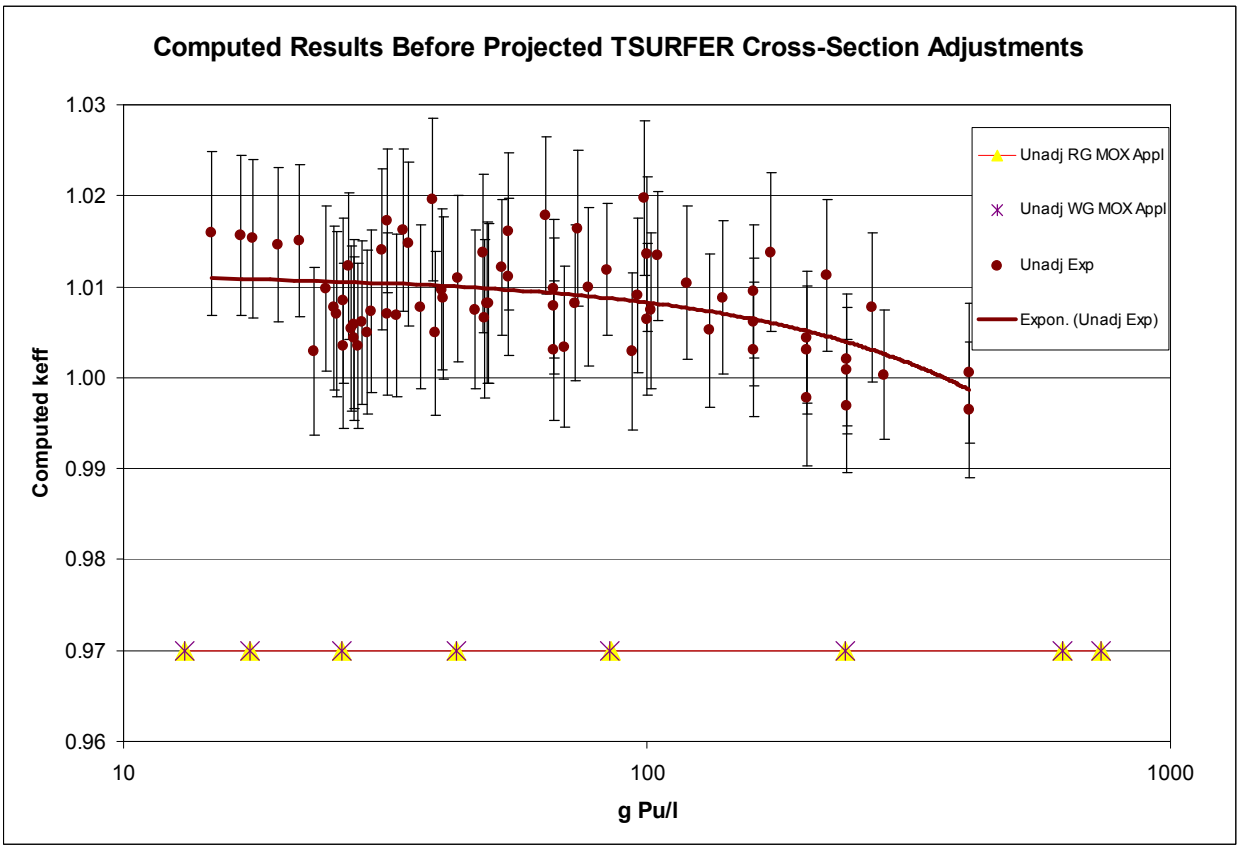

Figure 4. Computational results before projected adjustments

The TSURFER projected computational results following the benchmark uncertainty and covariance reevaluations, considering cross-section uncertainties and covariances to minimize the experimental and computed benchmark k_{eff} values, are provided in Figure 5.

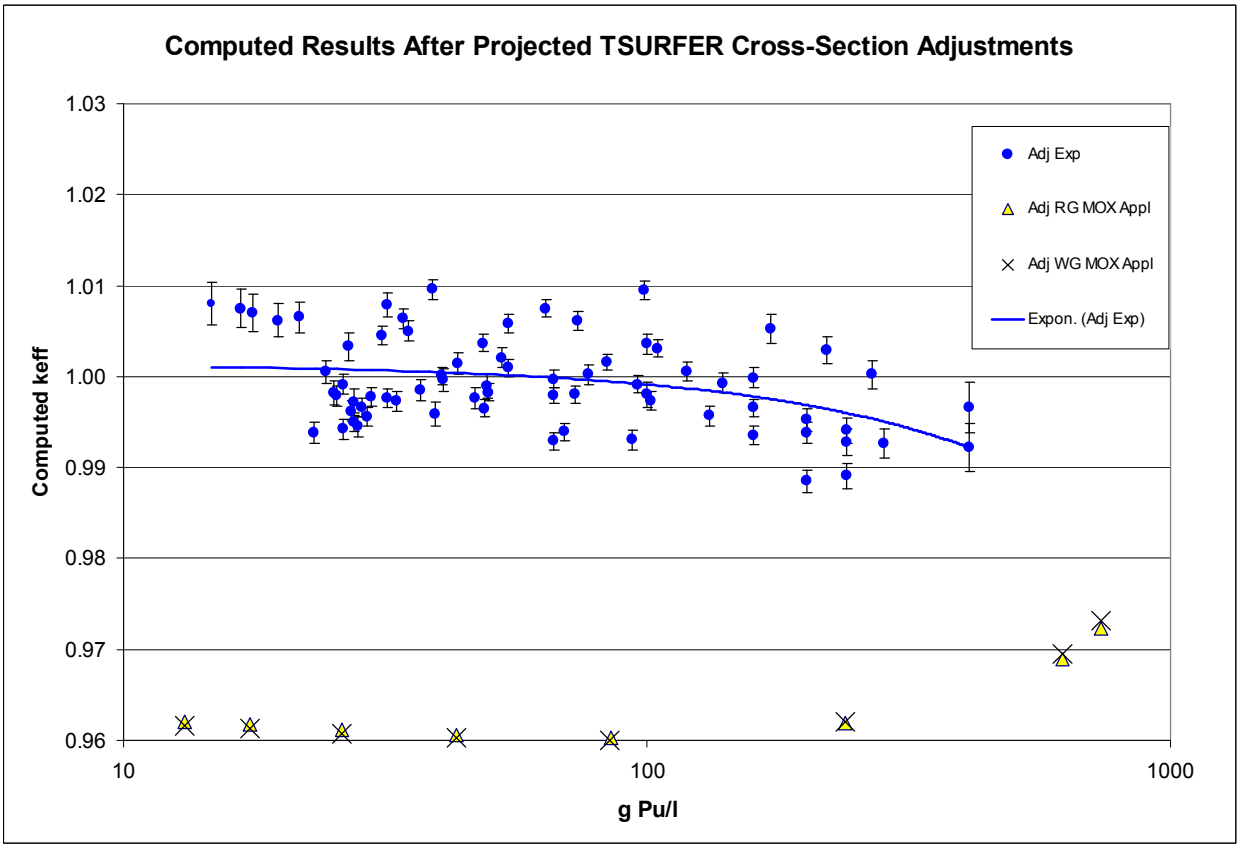

Figure 5. Computational results after projected adjustments

This is to say that if the cross-sections were modified according to this minimization process, the resultant computed values for the benchmarks and the RG and WG safety applications would be as shown in Figure 5.

An additional feature of the prototypic TSURFER code is that it can report the energy group-wise changes, in terms of fractional uncertainties, for neutron cross-section adjustments resulting from minimizing differences between calculated and experimental values of k_{eff}.

Summary

This study has presented summary results obtained from the Oak Ridge National Laboratory SCALE system prototypic computer code, TSURFER, for performing statistical analysis of water-moderated RG and WG plutonium selected "safety applications" by reevaluating and refining IHECSBE experimental uncertainties and covariances.

References

1. *International Handbook of Evaluated Criticality Safety Benchmark Experiments. Organization for Economic Cooperation and Development–Nuclear Energy Agency*, NEA/NSC/DOC(95)03 (September 2005 Edition).

2. Annual report on the ISTC Project 815.2, *Development of Computerized Technology for Criticality Safety Uncertainty Evaluation Based on the Analysis of Data of the International Bank on Critical Experiments*, Institute of Physics and Power Engineering, September 14, 2006.

3. SCALE 5.1, Computer Code Number : C00732, "Modular Code System for Performing Criticality and Shielding Analyses for Licensing Evaluation," Radiation Safety Information Computational Center, Oak Ridge National Laboratory, Oak Ridge, TN, USA.

4. M. L. Williams, B. L. Broadhead, and J. J. Wagschal, "An Adjustment Code to Determine Biases and Uncertainties in Nuclear System Responses by Consolidating Differential Data and Benchmark Integral Experiments," (Draft–August 11, 2005).