Data Adjustment Exercises for Fast Critical Benchmark Problems Using SCALE[1]

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INTRODUCTION

The Working Party on International Nuclear Data Evaluation Co-operation (WPEC) Subgroup 33 was established to study the use of integral experiments and covariance data for nuclear data adjustment and to recommend a set of best practices for improving evaluated nuclear data files [1]. In the Phase II Benchmark, participants are asked to calculate integral responses for several fast critical benchmark experiments and nuclear data sensitivity coefficients for these quantities. These sensitivity coefficients are used to guide the adjustment of nuclear data to minimize the difference between the calculated and experimental responses. This work summarizes the results of the Oak Ridge National Laboratory's (ORNL) participation in this data adjustment exercise using the sensitivity and uncertainty analysis capabilities of the SCALE code system [2] [3].

NUCLEAR DATA ADJUSTMENT METHODOLOGY

SCALE includes a generalized linear least-squares (GLLS) tool for data adjustment. Using sensitivity and uncertainty data, the GLLS procedure provides a consistent approach for "consolidating" integral benchmark measurements with calculated results to improve the final estimates for the response values. The procedure identifies a single set of adjustments to nuclear data, taking into account their correlated uncertainties as well as the experimental uncertainties. The resulting revised data will cause the computational models to produce response values that are as close as possible to experimental response values while also reducing response uncertainties. The responses examined during the data adjustment process are not limited to eigenvalue responses and can include a generalized set of responses such as reaction rate ratios, spectral indices, ratios of neutron fluxes, etc. Furthermore, these generalized responses can be calculated for single or multiple nuclides within a mixture and can use either microscopic or macroscopic cross sections. GLLS forces the adjusted calculated and measured responses to agree while constraining the data variations to minimize a generalized chi-squared parameter. The resulting nuclear data adjustments can provide guidance to evaluators interested in improving the differential data.

The TSUNAMI code suite can currently calculate eigenvalue and general response sensitivities for one-dimensional (1D) and two-dimensional (2D) (X-Y) systems and can calculate eigenvalue sensitivities for three-dimensional (3D) systems. The experiments analyzed in this benchmark data adjustment study included several 1D systems and several 2D, R-Z systems; the scope of ORNL's data adjustment exercise was limited to the 1D systems because of the lack of an R-Z or 3D generalized perturbation theory capability in SCALE.

Having generated eigenvalue and general response sensitivities, the SCALE TSUNAMI-1D analysis sequence stores these data in sensitivity data files (SDFs), which are then passed to the TSURFER (Tools for Sensitivity/Uncertainty analysis of Response Functions using Experimental Results) code, which executes the GLLS procedure.

TSURFER performs nuclear data adjustments with the target of moving the data points by no more than 1.2 standard deviations because very large, unrealistic data adjustments can indicate inconsistent or outlying experimental data. TSURFER also has a filtering method to ensure that no single experiment contributes too significantly to the calculated chi-square statistic. Although TSURFER contains several options for chi-square filtering, the "delta chi-square" method is the default chi-square filtering approach; this approach involves progressively omitting individual experiments from the data adjustment calculation to identify experiments that contribute excessively to the chi-square statistic [3] [4].

BENCHMARK PROBLEM DESCRIPTION

As shown in Table I, the WPEC Subgroup 33 benchmark problems consist of simplified models of seven fast critical benchmark systems [5]. Unfortunately four of the seven problems required the ability to calculate generalized responses in R-Z geometry, and thus the ORNL results for this benchmark study were limited to the Jezebel-Pu-239, Jezebel-Pu-240, and Flattop cases.

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Table I. WPEC Subgroup 33 Benchmark Problems

Benchmark Problem
Jezebel (Pu-239 configuration)
Jezebel (Pu-240 configuration)
Flattop (Pu-239 configuration)
ZPR6-7 (standard configuration)
ZPR6-7 (high Pu-240 content)
ZPPR-9
Joyo

The responses of interest in this benchmark study included the eigenvalue for each system and several spectral indices, as described in Table II. The spectral indices F28/F25, F49/F25, and F37/F25 represent the ratio of the fission rates for activation foils containing U-238, Pu-239, or Np-237, respectively, and a foil containing U-235.

Table II. Experimental Responses of Interest

Experiment	Responses
Jezebel-Pu239	k_{eff}
	F28/F25
	F49/F25
	F37/F25
Jezebel-Pu240	k_{eff}
Flattop	k_{eff}
	F28/F25
	F37/F25

Sensitivity coefficients were calculated for the benchmark problem responses of interest using TSUNAMI-1D with ENDF/B-VII.0 238-group cross sections and SCALE 6.1 44-group covariance data [3]. The experimental response covariance information used in this data adjustment exercise was generated by Ishikawa [6]. Effort is currently under way at ORNL to generate experimental correlation data for these and other experimental responses.

Direct perturbation calculations were performed to confirm the accuracy of the eigenvalue and general response sensitivity coefficients; these direct perturbation confirmations were limited to the most significant nuclides, which typically included Pu-239, Pu-240, and U-238. Plots of several sample sensitivity coefficient profiles are given in Figs. 1 and 2 for the Jezebel-Pu240 k_{eff} and Flattop F37/F25 responses, respectively. An S_{256} quadrature set was used for all sensitivity coefficient calculations.

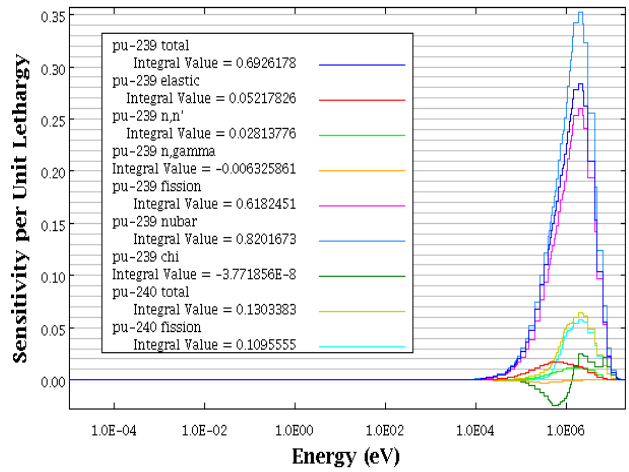

Fig. 1. Sample Jezebel-Pu240 k_{eff} sensitivities.

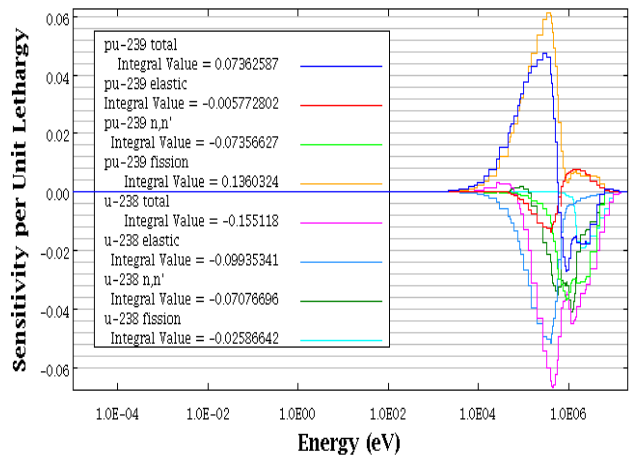

Fig. 2. Sample Flattop F37/F25 sensitivities.

DATA ADJUSTMENT RESULTS

Table III gives the initial calculated values, experimental values, and adjusted values for each of the response parameters. The C/E ratio is defined as ratio between the calculated and experimental value for some parameter; Table IV gives the initial and adjusted C/E ratios for the responses. None of the experimental responses were selected to be omitted during the adjustment process by the chi-square filtering method.

Table III. Initial, Experimental, and Adjusted Response Values

Experiment	Responses	Calc. Value	Exp. Value	Adj. Value
Jezebel-Pu239	k_{eff}	1.0000	1.0000	0.9996
	F28/F25	0.2086	0.2133	0.2134
	F49/F25	1.4243	1.4609	1.4393
	F37/F25	0.9714	0.9835	0.9774
Jezebel-Pu240	k_{eff}	1.0008	1.0000	1.0003
Flattop	k_{eff}	1.0026	1.0000	1.0005
	F28/F25	0.1746	0.1799	0.1789
	F37/F25	0.8477	0.8561	0.8549

Table IV. Initial and Adjusted C/E Values

Experiment	Responses	Initial C/E	Adjusted C/E
Jezebel-Pu239	k_{eff}	1.0000	0.9996
	F28/F25	0.9782	1.0006
	F49/F25	0.9749	0.9852
	F37/F25	0.9877	0.9938
Jezebel-Pu240	k_{eff}	1.0003	1.0003
Flattop	k_{eff}	1.0005	1.0005
	F28/F25	0.9946	0.9946
	F37/F25	0.9986	0.9986
Average C/E		**0.9881**	**0.9966**

As shown in Tables III and IV, the TSURFER data adjustment process produced an adjusted set of nuclear data that improved the accuracy of nearly all of the response parameters, with the exception being the Jezebel-Pu239 k_{eff}, which had an initial C/E of 1. The effectiveness of the data adjustment procedure is further highlighted by the fact that the value of the difference between the average C/E and one decreased by almost an order of magnitude after the data adjustment.

The GLLS data adjustment process also has the property of reducing the uncertainty in the calculated responses that is caused by uncertainty in the nuclear data. These adjusted responses have less uncertainty than the initial calculated responses because TSURFER has essentially validated them against the experimental data. Table V compares the relative uncertainty for the experimental responses, the initial calculated responses, and the adjusted responses, and shows the amount of the uncertainty reduction observed. As shown in Table V, the GLLS process significantly reduces the amount of uncertainty in the calculated responses; the amount of uncertainty reduction ranged from 32.6% to 87.5%, with an average drop in uncertainty of 77.0%.

Table V. Effect of the Nuclear Data Adjustment on the Response Uncertainties

Exp.	Resp.	Exp. Unc.	Calc. Unc.	Adj. Unc.	Unc. Reduct.
Jezebel-Pu239	k_{eff}	0.20%	1.39%	0.17%	87.5%
	F28/F25	1.10%	4.11%	0.85%	79.3%
	F49/F25	0.90%	0.81%	0.54%	32.6%
	F37/F25	1.40%	7.49%	1.01%	86.6%
Jezebel-Pu240	k_{eff}	0.20%	1.21%	0.17%	85.9%
Flattop	k_{eff}	0.30%	1.25%	0.25%	79.7%
	F28/F25	1.10%	3.67%	0.81%	78.0%
	F37/F25	1.40%	7.40%	1.00%	86.4%

Figure 3 shows the nuclear data adjustments computed by TSURFER for the most significantly adjusted cross sections. As shown in Fig. 3, the elastic and (n,n′) reactions realized the largest amount of adjustment, while the fission and capture cross sections saw relatively small adjustments. The relatively insignificant adjustments that were required for the fission and capture cross sections may be a result of the non-thermal nature of the problem, or may arise from the difficulty involved in accurately calculating cross sections for inelastic scattering reactions.

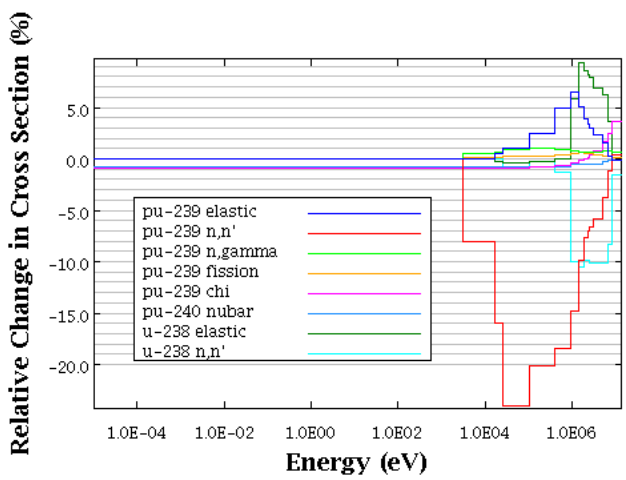

Fig. 3. TSURFER predicted nuclear data adjustments.

Lastly, the TSURFER calculation was repeated using either the eigenvalue response information or the spectral index response information. Figure 4 compares the predicted adjustment for the most significantly adjusted nuclides using only the eigenvalue (keff) and spectral index (GPT) data with the adjustment that is predicted using the complete set of data. As shown in Fig. 4, comparing only the calculated and experimental eigenvalue information does not result in an accurate

estimate of the full set of data adjustments. This suggests that nuclear data adjustment exercises might need to include generalized responses in their analysis to accurately guide adjustments in nuclear data; a more thorough investigation covering more experiments is needed to support this hypothesis.

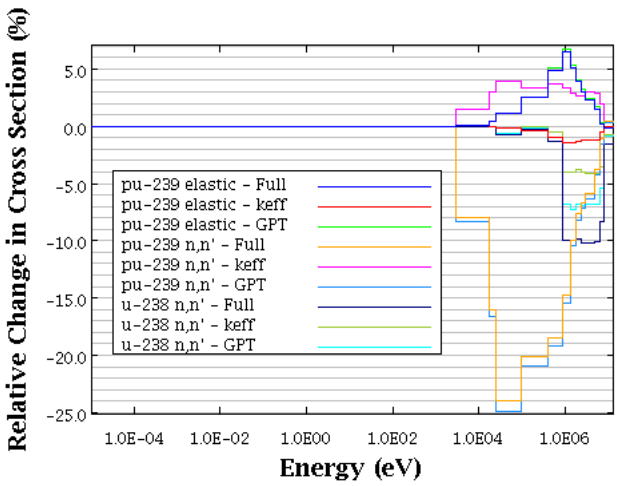

Fig. 4. Comparison of TSURFER predicted data adjustments with and without the use of generalized responses.

CONCLUSIONS

The TSUNAMI methodology for nuclear data adjustment has been applied to several test problems within the scope of the WPEC Subgroup 33 mission. The TSUNAMI-1D code predicted accurate sensitivity coefficients for the test problems, and these sensitivity coefficients were used by the TSURFER code to adjust the nuclear data to minimize the difference between the calculated and experimental responses of interest. The TSURFER data adjustment significantly improved the C/E values for the different responses, and the ^{239}Pu, ^{240}Pu, and ^{238}U elastic and inelastic cross sections were affected the most by this adjustment. The GLLS data adjustment process also significantly reduced the amount of uncertainty of the calculated responses that is due to uncertainty in the nuclear data, and produced an average response uncertainty reduction of 77.0%.

This data adjustment exercise was repeated using only eigenvalue response data, and the nuclear data adjustments from this exercise were shown to differ significantly from those using the complete set of experiment response data. This suggests that a generalized set of responses might need to be included in data adjustment exercises to obtain a complete estimate of the necessary data adjustments. Future work includes developing a generalized perturbation capability in TSUNAMI-3D to calculate these general responses for more complex systems, and expanding the scope of this study to span many other systems, including several challenge problems with C/E values that are not close to unity.

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REFERENCES

1. E. DUPONT, G. PALMIOTTI, M. SALVATORES, "Working Party on International Nuclear Data Evaluation Co-operation (WPEC) Subgroup 33." 29 May 2012. Retrieved from http://www.oecd-nea.org/science/wpec/sg33/
2. "SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design," ORNL/TM-2005/39, Version 6.1, Oak Ridge National Laboratory, Oak Ridge, Tennessee (June 2011). Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-785.
3. B. T. REARDEN et al., "Sensitivity and Uncertainty Analysis Capabilities and Data in SCALE," *Nucl. Technol.*, **174**, 236–288 (2011).
4. Y. YEIVIN, J. J. WAGSCHAL, J. H. MARABLE, and C. R. WEISBIN, "Relative Consistency of ENDF/B-IV and –V with Fast Reactor Benchmarks," *Proc. Int. Conf. on Nuclear Cross Sections for Technology*, J. L. Fowler, C. H. Johnson, and C. D. Bowman, eds., NBS SP 594 (1980).
5. *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, Nuclear Energy Agency Nuclear Science Committee of the Organization for Economic Co-operation and Development, NEA/NSC/DOC(95)03, Paris (2010).
6. M. ISHIKAWA, "How to Determine Error Matrix of Integral Data," Japan Atomic Energy Agency, Ibaraki 319-1195, Japan (November 2011). Retrieved from http://www.oecd-nea.org/science/wpec/sg33/6th_meeting/5_Report_on_Integral_Error_Matrix_20111125.pdf