Uncertainty Quantification Techniques of SCALE/TSUNAMI*

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INTRODUCTION

The Standardized Computer Analysis for Licensing Evaluation (SCALE) code system [1] developed at Oak Ridge National Laboratory (ORNL) includes Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI).[2] The TSUNAMI code suite can quantify the predicted change in system responses, such as k_{eff}, reactivity differences, or ratios of fluxes or reaction rates, due to changes in the energy-dependent, nuclide-reaction-specific cross-section data.

Where uncertainties in the neutron cross-section data are available, the sensitivity of the system to the cross-section data can be applied to propagate the uncertainties in the cross-section data to an uncertainty in the system response. Uncertainty quantification is useful for identifying potential sources of computational biases and highlighting parameters important to code validation.

Traditional validation techniques often examine one or more average physical parameters to characterize a system and identify applicable benchmark experiments. However, with TSUNAMI correlation coefficients are developed by propagating the uncertainties in neutron cross-section data to uncertainties in the computed responses for experiments and safety applications through sensitivity coefficients. The bias in the experiments, as a function of their correlation coefficient with the intended application, is extrapolated to predict the bias and bias uncertainty in the application through trending analysis or generalized linear least squares techniques, often referred to as "data adjustment."

Even with advanced tools to identify benchmark experiments, analysts occasionally find that the application models include some feature or material for which adequately similar benchmark experiments do not exist to support validation. For example, a criticality safety analyst may want to take credit for the presence of fission products in spent nuclear fuel. In such cases, analysts sometimes rely on "expert judgment" to select an additional administrative margin to account for gap in the validation data or to conclude that the impact on the calculated bias and bias uncertainty is negligible. As a result of advances in computer programs and the evolution of cross-section covariance data, analysts can use the sensitivity and uncertainty analysis tools in the TSUNAMI codes to estimate the potential impact on the application-specific bias and bias uncertainty resulting from nuclides not represented in available benchmark experiments. This paper presents the application of methods described in a companion paper.[3]

SENSITIVITY DATA

The basis of the TSUNAMI validation techniques is that computational biases are primarily caused by errors in the cross-section data, which are quantified and bounded by the cross-section-covariance data. To provide credence to this claim, sensitivity data for 281 critical benchmark experiments were generated with TSUNAMI-3D, and the cross-section-covariance data were propagated to uncertainties in the computed values of k_{eff}.

It is important to model an experiment with the computer code the way it is evaluated into a benchmark so that the performance of the code and the associated cross-section libraries may be determined accurately within the uncertainties of both the benchmark evaluation and the computational results. As such, the models and data used in this analysis were drawn from the SCALE Verified, Archived, Library of Inputs and Data (VALID).[4] The SCALE VALID procedure provides a quality assurance framework for preparing, reviewing, and storing input models and data sets computed from the models so that one can use the models and data in analyses with confidence. The procedure ensures that the models and data were correctly generated using appropriate references with documented checks and reviews. Configuration management is implemented to prevent inadvertent modification of the models and data or inclusion of models that have not undergone the rigorous review process. The VALID models and sensitivity data are distributed annually through the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (IHECSBE).[5]

SCALE CROSS-SECTION COVARIANCE DATA

Once quality-assured sensitivity data are available, the TSUNAMI tools that perform uncertainty analysis require reasonable estimates for nuclear data uncertainties. Historically, the lack of sufficient covariance information in nuclear data files such as ENDF/B has limited the usefulness of tools like TSUNAMI. The SCALE 6 cross-section covariance library is a single comprehensive library with a total of 401 materials in the SCALE 44-energy-group structure.[1,2] The SCALE covariance library data correspond to 44-group relative uncertainties assembled from a variety of sources, including evaluations from ENDF/B-VII, ENDF/B-VI, JENDL-3.1, and more than 300 approximated uncertainties from a collaborative project performed by Brookhaven National Laboratory, Los Alamos National Laboratory, and ORNL.[1,2]

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Because SCALE includes separate multigroup cross-section libraries processed from ENDF/B-V, ENDF/B-VI.8, and ENDF/B-VII.0, the application of a single "generic" covariance library to all multigroup cross-section libraries obviously raises questions about consistency with any given data evaluation. In reality much of the approximate uncertainty data in the library is based on simplifying approximations that do not depend on specific ENDF evaluations and thus can be applied to all cross-section libraries within the limitations of the assumed methodology. In other cases where a covariance evaluation has been taken from a specific nuclear data file (e.g., ENDF/B-VII, ENDF/B-VI, or JENDL-3.1), it is assumed that the same *relative* (rather than *absolute*) uncertainties can be applied to all cross-section libraries, even if these are not strictly consistent with the nuclear data evaluations. This may be questionable for some older evaluations in the ENDF/B-V data, but it should be reasonable for the SCALE ENDF/B-VI and VII cross-section libraries. The assumption is partially justified by the fact that different evaluations often use many of the same experimental measurements, since there is a limited amount of this information available. Also, because most important nuclear data are now known rather well, newer evaluations in many instances correspond to rather modest variations from previous ones and are expected to lie within the earlier uncertainties.

It should be noted that there is no inherently "true" uncertainty that can be defined unambiguously for nuclear data. While differences in nuclear data evaluations have direct impact on calculations that can be affirmed by comparisons with benchmark experiments, it is more difficult to quantify the reliability of uncertainty estimates. In general, the SCALE covariance library should be viewed as a best-estimate assessment of data uncertainties. Nevertheless, it is felt that the SCALE covariance library is a reasonable representation of the nuclear data uncertainties, given the current lack of information. The usefulness of these data uncertainties is demonstrated in a subsequent section.

UNCERTAINTY ANALYSIS RESULTS

Application of these covariance data to 281 benchmark experiments, consisting of a variety of fuel types and moderation levels, results in the k_{eff} plots shown in Fig. 1 for high-enriched uranium (HEU), intermediate-enriched uranium (IEU), low-enriched uranium (LEU), mixed-oxide (MOX), and plutonium (PU) fuel types. The fuel forms represented are heterogeneous compounds (COMP) such as fuel rod arrays, metal (MET), and fissile solutions (SOL) with neutron spectra classified as fast (FAST) and thermal (THERM). Each system is modeled with SCALE 6 using ENDF/B-VII cross-section data in the 238-group energy structure. In Fig. 1, the actual computational biases of the benchmarks are shown as deviation of the computed-to-experimental result ratio (C/E) from unity. The experimental uncertainty for each benchmark is shown as a dashed line, and the uncertainty due to cross-section covariance data is shown as a solid line. Analysis of the distribution of data in Fig. 1 reveals that computed and experimental values agree within one standard deviation due to covariance data for 97% of the experiments, within two standard deviations for 99.6%, and within three standard deviations for 100%. Thus, with few exceptions the TSUNAMI data shown in Fig. 1 demonstrate that the uncertainties associated with the nuclear data bound the actual observed biases for the 281 systems of various fuel types and moderation levels examined.

CONCLUSIONS

The results presented here demonstrate the usefulness of the TSUNAMI sensitivity and uncertainty analysis methods and data to provide bounding estimates for computational biases for a variety of benchmark experiments. The uncertainty values provided by TSUNAMI are demonstrated to provide bounding estimates for actual computational biases for 281 benchmark experiments with a variety of fuel types and spectra. Sensitivity and uncertainty analysis techniques such as trending on correlation coefficients and application of generalized linear least squares techniques can be implemented as advanced validation techniques. Additionally, uncertainty analysis can applied conservatively to supplement validation techniques where applicable benchmark experiments are not available to provide full validation coverage for a system of interest.

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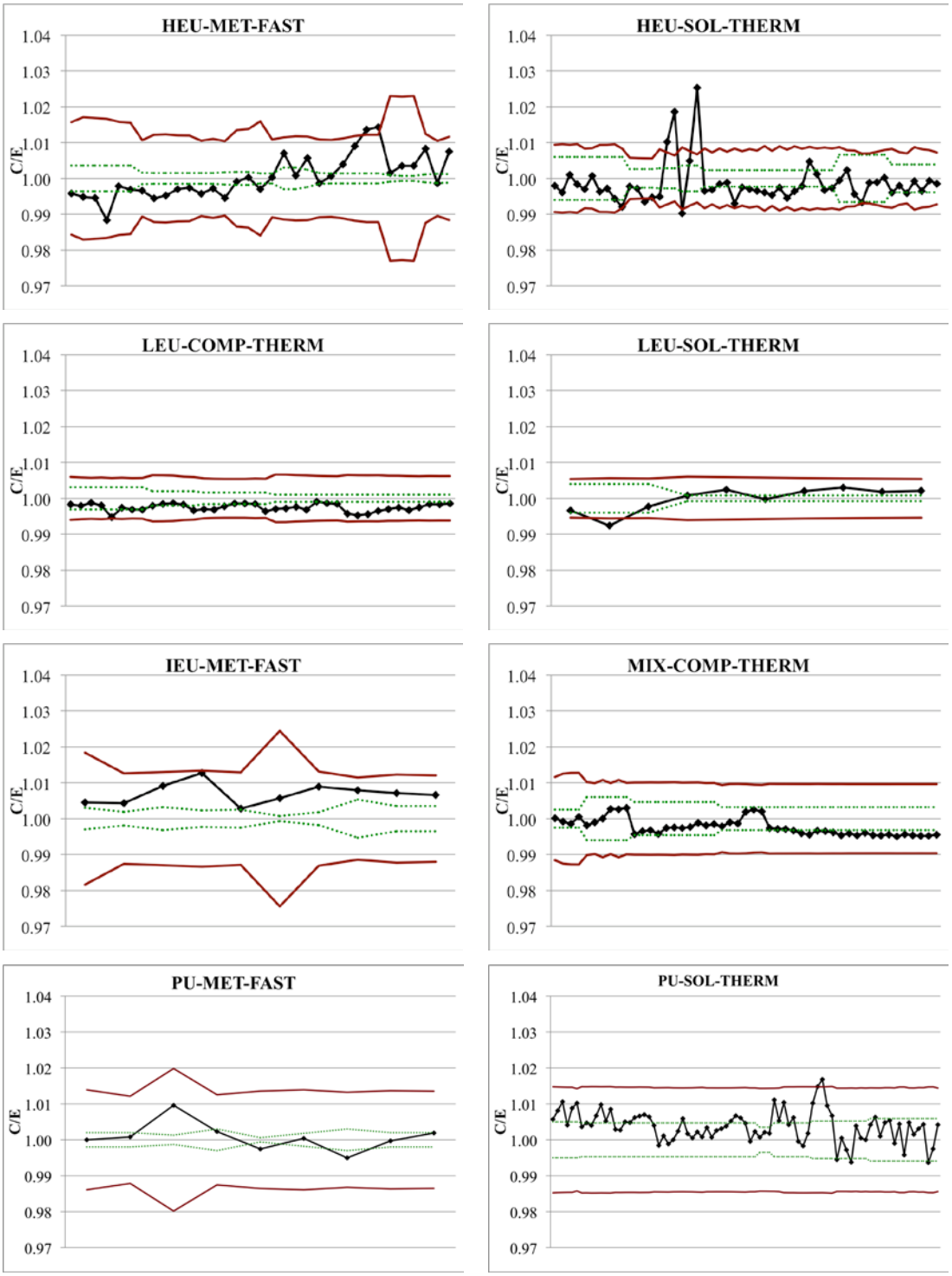

Fig. 1: C/E, experimental uncertainty (dotted line), and cross-section uncertainty (solid line) for benchmark experiments.