SCALE/TSUNAMI SENSITIVITY DATA FOR ICSBEP EVALUATIONS*

B. T. Rearden, D. A. Reed, R. A. Lefebvre, D. E. Mueller, and W. J. Marshall

Oak Ridge National Laboratory
P.O. Box 2008, Bldg. 5700, Oak Ridge, TN 37831-6170, USA
ReardenB@ornl.gov

ABSTRACT

The Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) software developed at Oak Ridge National Laboratory (ORNL) as part of the Scale code system provide unique methods for code validation, gap analysis, and experiment design. For TSUNAMI analysis, sensitivity data are generated for each application and each existing or proposed experiment used in the assessment. The validation of diverse sets of applications requires potentially thousands of data files to be maintained and organized by the user, and a growing number of these files are available through the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (IHECSBE) distributed through the International Criticality Safety Benchmark Evaluation Program (ICSBEP). To facilitate the use of the IHECSBE benchmarks in rigorous TSUNAMI validation and gap analysis techniques, ORNL generated SCALE/TSUNAMI sensitivity data files (SDFs) for several hundred benchmarks for distribution with the IHECSBE. For the 2010 edition of IHECSBE, the sensitivity data were generated using 238-group cross-section data based on ENDF/B-VII.0 for 494 benchmark experiments. Additionally, ORNL has developed a quality assurance procedure to guide the generation of Scale inputs and sensitivity data, as well as a graphical user interface to facilitate the use of sensitivity data in identifying experiments and applying them in validation studies.

Key Words: ICSBEP, TSUNAMI, sensitivity, validation

1 INTRODUCTION

The Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) software developed at Oak Ridge National Laboratory (ORNL) as part of the Scale code system provides a unique means of determining the similarity of nuclear criticality experiments to safety applications[1]. Instead of using an average physical parameter (such as the H/X ratio or EALF) to characterize a system, correlation coefficients are developed by propagating the uncertainties in neutron cross-section data to uncertainties in the computed neutron multiplication factor for experiments and safety applications via sensitivity coefficients. The bias in the experiments, as a function of correlation with the intended application, is extrapolated to predict the bias and bias uncertainty in the application. Additionally, TSUNAMI includes the data adjustment tool, TSURFER (Tool for Sensitivity/Uncertainty Analysis of Response Functions using Experimental Results), which can assimilate biases from many different sources to project the bias and bias uncertainty of an application.

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For TSUNAMI analysis, sensitivity data are generated for each application and each experiment used in the validation. The validation of diverse sets of applications requires potentially thousands of data files to be maintained and organized by the user, and a growing number of these files are available through the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (IHECSBE) distributed through the International Criticality Safety Benchmark Evaluation Program (ICSBEP)[2]. To facilitate the use of the IHECSBE benchmarks in rigorous TSUNAMI validation techniques, ORNL generated SCALE/TSUNAMI sensitivity data files (SDFs) for several hundred benchmarks for distribution with the IHECSBE. For the 2010 edition of IHECSBE, the sensitivity data were generated using 238-group cross-section data based on ENDF/B-VII.0. The direct implementation of these SDFs into any safety application, including applicable Quality Assurance procedures, is the responsibility of the organization performing the safety analysis. The SDFs included on the IHECSBE provide, at the minimum, a broad set of sensitivity data for critical experiments that should provide the basis for a rigorous validation. In non-safety applications, the SDFs provided can be used within the TSUNAMI tool suite to perform a wide range of analyses as discussed in more detail below. Additionally, ORNL has developed a graphical user interface to facilitate the use of sensitivity data in identifying experiments and applying them in validation studies.

2 APPLICATIONS OF SENSITIVTY AND UNCERTAINTY DATA

The TSUNAMI software provides a unique means of determining the similarity of nuclear criticality experiments to safety applications.[3] The basis of the TSUNAMI validation techniques is the assumption that computational biases are primarily caused by errors in the cross-section data, the potential for which are quantified in cross-section-covariance data. To determine the bias in a given safety system using these advanced techniques, the sensitivity of k_{eff} to the cross-section data must be known not only for the safety system, but also for all benchmark experiments considered in its validation.

2.1 Sensitivity Coefficient Generation

The TSUNAMI-1D and TSUNAMI-3D analysis sequences compute the sensitivity of k_{eff} to energy-dependent cross-section data for each reaction of each nuclide in a system model. The one-dimensional (1D) transport calculations are performed with XSDRNPM, and the three-dimensional (3D) calculations are performed with KENO V.a or KENO-VI. The energy-dependent sensitivity data are stored in an SDF for subsequent analysis. Additionally, the TSUNAMI-1D and -3D sequences compute the uncertainty in each system's k_{eff} value due to the cross-section-covariance data.

TSAR (Tool for Sensitivity Analysis of Reactivity Responses) computes the sensitivity of the reactivity change between two k_{eff} calculations, using SDFs from TSUNAMI-1D and/or TSUNAMI-3D. TSAR also computes the uncertainty in the reactivity difference due to the cross-section-covariance data.

2.2 Bias and Bias Uncertainty Assessment

TSUNAMI provides two tools to establish the computational bias introduced through cross-section data. TSUNAMI-IP (TSUNAMI Indices and Parameters) uses the SDFs generated from TSUNAMI-1D, -3D, or TSAR for a series of systems to compute correlation coefficients that determine the amount of shared uncertainty between each target application and each benchmark experiment considered in the analysis. TSURFER (Tool for S/U Analysis of Response Functions Using Experimental Results) is a bias and bias uncertainty

prediction tool that implements the generalized linear least-squares (GLLS) approach to data assimilation and cross-section data adjustment.

Instead of using one or more average physical parameters to characterize a system, TSUNAMI-IP determines the uncertainty in k_{eff}, due to cross-section uncertainties that is shared between two systems. This shared uncertainty in k_{eff} directly relates to the bias shared by the two systems and is identified as the correlation coefficient for k_{eff} denoted as c_k. The TSUNAMI validation techniques, including the computation of c_k, require the sensitivity of k_{eff} to each group-wise nuclide-reaction-specific cross section for all systems considered in the analysis. Correlation coefficients are developed by propagating the uncertainties in neutron cross-section data to uncertainties in the computed neutron multiplication factor for experiments and safety applications through sensitivity coefficients. The bias in the experiments, as a function of correlated uncertainty with the intended application, is extrapolated to predict the bias and bias uncertainty in the target application. This correlation coefficient extrapolation method is useful where many experiments with uncertainties that are highly correlated to the target application are available.

The data adjustment or data assimilation techniques of TSURFER predict computational biases for general responses, including but not limited to k_{eff} .[3] The technique utilizes S/U data to identify a single set of adjustments to nuclear data and experimental responses, taking into account their correlated uncertainties, that will result in the computational models producing response values close to their experimental response value. Then the same data adjustments are used to predict an unbiased response (e.g., k_{eff}) value for the application and an uncertainty on the adjusted response value. The difference between the originally calculated response value and the new post-adjustment response value represents the bias in the original calculation, and the uncertainty in the adjusted value represents the uncertainty in this bias. If experiments are available to validate the use of a particular nuclide in the application, the uncertainty of the bias for this nuclide may be reduced. If similar experiments are not available, the uncertainty in the bias for the given nuclide is high. Thus, with a complete set of experiments to validate important components in the application, a precise bias with a small uncertainty can be predicted. Where the experimental coverage is lacking, a bias can be predicted with an appropriately large, application-specific, uncertainty. The data assimilation method presents many advantages over other techniques in that biases can be projected from an agglomeration of benchmark experiments, each of which may represent only a small component of the bias of the target application. Also, contributors to the computational bias, or gaps in validation due to lack of available experiments, can be analyzed on an energy-dependent, nuclide-reaction-specific basis.

2.3 Experiment Design

Where gaps in benchmark coverage are found, resulting in unacceptably high bias uncertainties, the TSUNAMI techniques can be applied in the design of optimized experiments to fill the gaps.[4] The techniques for similarity assessment can be applied to proposed experiment designs to quantify their similarity to the targeted application. The comparisons can be based on the similarity of individual sensitivity profiles or in terms of global similarity using c_k.

In many cases, it is not practical to assemble a benchmark experiment that would produce a high c_k relative to a given application. In these cases, it may be possible to use reactivity experiments, where a single test material produces sensitivities in a similar spectrum as the application, and then carefully design a reference experiment without the test material. If the sensitivities for materials other than the test material are closely matched

between the test experiment and the reference experiment, TSAR and TSURFER can be applied to extract the bias due just to the test material and project it to a bias for the same material in the application system.

The TSUNAMI assessment of validation gaps and the design of experiments to fill those gaps is a required step in the US Department of Energy (DOE) Nuclear Criticality Safety Program (NCSP) C_EdT (Critical and Sub-critical Experiment Design Team) process. However, before gaps in existing experiments can be identified, sensitivity data must be available for existing experiments.

3 VERIFIED, ARCHIVED LIBRARY OF INPUTS AND DATA

To facilitate the application of TSUNAMI methodologies to advanced validation and C_EdT, Scale input files and SDFs have been generated as part of an effort jointly supported by the NCSP and the US Nuclear Regulatory Commission (NRC). Files generated under this project follow the quality assurance procedure for the generation of a Verified, Archived Library of Input and Data (VALID)[5]. The VALID procedure requires input models to match the description provided in the Benchmark Specifications section of an IHECSBE benchmark evaluation to the extent possible using multi-group cross sections and three-dimensional modeling with KENO V.a or KENO-VI. The models are generated by an expert originator and independently checked by an expert reviewer. Additionally, the sensitivity data generated through TSUNAMI calculations are rigorously checked with direct perturbation calculations to ensure the data accurately represent the expected response of k_{eff} to changes in the cross-section data. Models are often refined after direct perturbation results reveal inadequate resonance self-shielding models or inadequate spatial resolution of the flux solution as demonstrated through the use of mesh flux accumulators. The input models and sensitivity results are only accepted into the VALID archive for eventual distribution with the IHECSBE after they have passed this rigorous assessment of quality by the originator and reviewer, as approved by the VALID Quality Assurance Coordinator.

4 SENSITIVITY DATA DISTRIBUTED IN THE IHECSBE

For the 2010 distribution of the IHECSBE (the current version as of this writing), the US NRC provided support to generate new benchmark models and data under the VALID process. When added to the VALID benchmarks provided in 2009, a total of 245 VALID benchmarks are provided in the 2010 IHECSBE. The benchmark cases are summarized in Table 1. Note that in some cases the SDF name differs from the stated evaluation name and case identifier. These differences are due to cross-referenced cases in the IHECSBE, where a benchmark from one evaluation may be documented in another evaluation, effectively providing two identifiers for a benchmark.

The TSUNAMI sensitivity data are located in the directories `Dice/data/ornl/TSUNAMI-1D` and `Dice/data/ornl/TSUNAMI-3D`. Input files for systems that have passed through the VALID process are also distributed in `Dice/data/ornl/inputs` for both TSUNAMI and Criticality Safety Analysis Sequences (CSAS) of SCALE. Where detailed and simplified models are described for a benchmark and both the detailed and simplified input models are provided, the SDFs are only provided for the detailed models. In some cases, only the simplified model is provided. The simplified inputs and SDFs are denoted with an “S” at the end of the filename, as in *HEU-MET-FAST-018-001S.inp*, for example.

Table 1. Benchmarks with inputs and SDFs generated through the VALID process

Evaluation	Cases
HEU-MET-FAST-005	1–6
HEU-MET-FAST-008	1
HEU-MET-FAST-009	1–2
HEU-MET-FAST-010	1–2
HEU-MET-FAST-011	1
HEU-MET-FAST-013	1
HEU-MET-FAST-015*	1
HEU-MET-FAST-016	1–2
HEU-MET-FAST-017	1
HEU-MET-FAST-018	1
HEU-MET-FAST-019	1
HEU-MET-FAST-020	1
HEU-MET-FAST-021	1
HEU-MET-FAST-024	1
HEU-MET-FAST-025*	1–5
HEU-MET-FAST-030	1
HEU-MET-FAST-038	1–2
HEU-MET-FAST-040*	1
HEU-MET-FAST-065*	1
HEU-MET-FAST-080*	1
HEU-SOL-THERM-001	1–10
HEU-SOL-THERM-013	1–4
HEU-SOL-THERM-014	1–3
HEU-SOL-THERM-016	1–3
HEU-SOL-THERM-028	1–18
HEU-SOL-THERM-029	1–7
HEU-SOL-THERM-030	1–7
IEU-MET-FAST-002*	1
IEU-MET-FAST-003	1
IEU-MET-FAST-004	1
IEU-MET-FAST-005	1
IEU-MET-FAST-006*	1
IEU-MET-FAST-007*	1
IEU-MET-FAST-008*	1
IEU-MET-FAST-009	1
IEU-MET-FAST-019*	1–2
LEU-COMP-THERM-001	1–8
LEU-COMP-THERM-002	1–5
LEU-COMP-THERM-042*	1–7
LEU-COMP-THERM-050*	1–18
LEU-SOL-THERM-002	1–3
LEU-SOL-THERM-003	1–9
LEU-SOL-THERM-004	1–7
MIX-COMP-THERM-001	1–4
MIX-COMP-THERM-002*	1–6

Evaluation	Cases
MIX-COMP-THERM-004	1–11
PU-MET-FAST-001	1
PU-MET-FAST-002	1
PU-MET-FAST-005*	1
PU-MET-FAST-006	1
PU-MET-FAST-008	1
PU-MET-FAST-010	1
PU-MET-FAST-018	1
PU-MET-FAST-022	1
PU-MET-FAST-023	1
PU-MET-FAST-024	1
PU-SOL-THERM-001	1–6
PU-SOL-THERM-002	1–7
PU-SOL-THERM-003	1–8
PU-SOL-THERM-004	1–13
PU-SOL-THERM-005*	9
PU-SOL-THERM-006*	3
PU-SOL-THERM-007*	8
PU-SOL-THERM-011*	1–8

*Benchmarks added for 2010.

Additional SDFs available in the IHECSBE were generated as part of a study published as *Application of the SCALE TSUNAMI Tools for the Validation of Criticality Safety Calculations Involving* ^{233}U, ORNL/TM-2008/196[6]. These input files were generated by expert users of Scale, but were generated before the formal VALID procedure was available. The data from the 249 benchmark models from ORNL/TM-2008/196 were generated with SCALE 6.0 using ENDF/B-VII.0 cross sections, where the original report used SCALE 5.1 with different cross sections. These benchmark cases are summarized in Table 2. Combining these with the benchmarks from VALID, a total of 494 SDFs are provided in the 2010 IHECSBE.

Table 2. Benchmarks with SDFs generated for ORNL/TM-2008/196

Evaluation	Cases
LEU-COMP-THERM-049	1–18
MIX-COMP-FAST-001	1
U233-COMP-THERM-001	2–4
U233-MET-FAST-001	1
U233-MET-FAST-002	1–2
U233-MET-FAST-003	1–2
U233-MET-FAST-005	1–2
U233-MET-FAST-006	1
U233-SOL-INTER-001	1–13, 15, 17–26, 28–29, 31–33
U233-SOL-MIXED-001	14, 16, 30
U233-SOL-MIXED-002	3, 5–6, 8–9
U233-SOL-THERM-001	1–5
U233-SOL-THERM-002	1–17
U233-SOL-THERM-003	1–10
U233-SOL-THERM-004	1–8
U233-SOL-THERM-005	1–2
U233-SOL-THERM-006	1–25
U233-SOL-THERM-008	1
U233-SOL-THERM-009	1–4
U233-SOL-THERM-011	27
U233-SOL-THERM-012	1–8
U233-SOL-THERM-013	1–21
U233-SOL-THERM-014	1–16
U233-SOL-THERM-015	1–2, 4, 7, 10–31
U233-SOL-THERM-016	1–4, 6–19, 21–33
U233-SOL-THERM-017	1–7

5 VIBE

To help streamline use of sensitivity data in the code validation process, the software package VIBE (Validation, Interpretation and Bias Estimation) was developed at ORNL as a component of Scale.[7] VIBE works as a stand-alone application distributed with Scale and also as a plug-in to DICE (Database for the International Handbook of Evaluated Criticality Safety Benchmark Experiments) as part of the 2010 IHECSBE. VIBE will scan a computer file system and locate all available TSUNAMI SDFs, which can include sensitivity data for the user's application as well as files from the IHECSBE. Because an SDF can contain millions of data points, VIBE helps the user consolidate these points by collapsing the data along one dimension (energy), and then allowing the user to sort and filter the data along other dimensions (nuclide, reaction, sensitivity values, etc). Once the data points are parsed with VIBE, the user can select the benchmarks most similar to the application based on sensitivity criteria. Lists of matching files can be stored in groups and passed to the Scale ExSITE (Extensible Scale Intelligent Text Editor) input generator, where the TSUNAMI validation analysis is conducted. VIBE is also capable of querying the DICE database distributed with the ICSBEP handbook to display the characteristic parameters of each benchmark (enrichment, EALF, H/X, etc.) along with the experimental and computed k_{eff} values and uncertainties in a tabular format. These data can be exported for further analysis,

such as traditional trending analysis with USLSTATS[8] and for comparison with the TSUNAMI results.

To access DICE with the VIBE plug-in activated, simply browse the 2010 IHECSBE to `/Handbook/plugins/Vibe` and launch DICE using the `vibe-dice.bat` or `vibe-dice.sh` scripts. VIBE will load on the far right tab of DICE, as shown in Figure 1. Note that several seconds may be required for VIBE to process the sensitivity data files on the DVD. Better performance will be obtained by copying the contents of the DVD to a local hard drive.

As shown in Figure 1, the 238-group ENDF/B-VII.0 TSUNAMI sensitivity data generated at ORNL can be accessed in `/Handbook/Dice/data/ornl/TSUNAMI-1D` and `TSUNAMI-3D`. The sensitivity data in the `/Handbook/Dice/data/sensitivity` directory were generated by the Institute of Physics and Power Engineering (IPPE) in Russia using their codes and 30-group ABBN-93 cross section data.

Specific step-by-step instruction on using VIBE to search for benchmarks using sensitivity criteria are provided in *Getting Started with VIBE as a DICE Plug-in Module*[7], which is also included in the IHECSBE DVD in `/Handbook/Dice/plugins/Vibe` directory. As an example, VIBE can be quickly used to identify experiments with the highest sensitivity to ^{149}Sm (n,gamma) at thermal energies, as shown in Figure 2. These experiments could be used directly in TSUNAMI studies, following instructions provided in *TSUNAMI Primer: A Primer for Sensitivity/Uncertainty Calculations with SCALE*.[9]

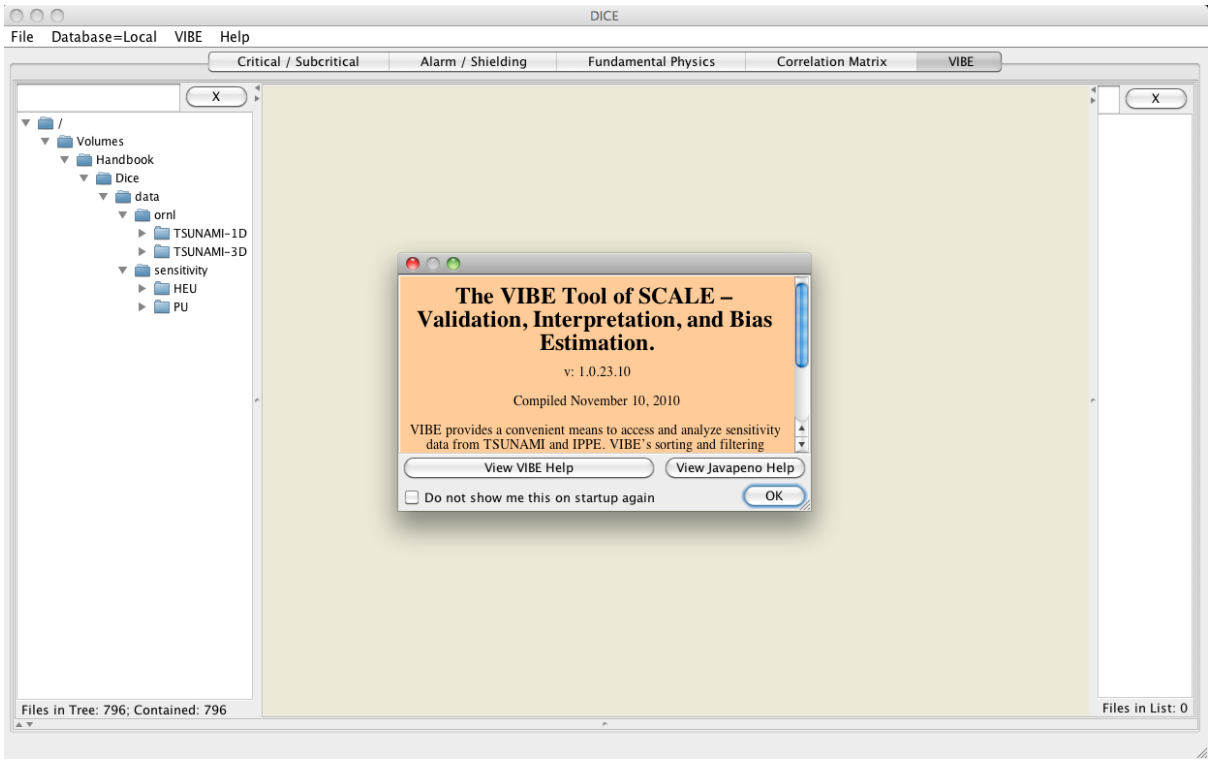

Figure 1. VIBE as a DICE plug-in module.

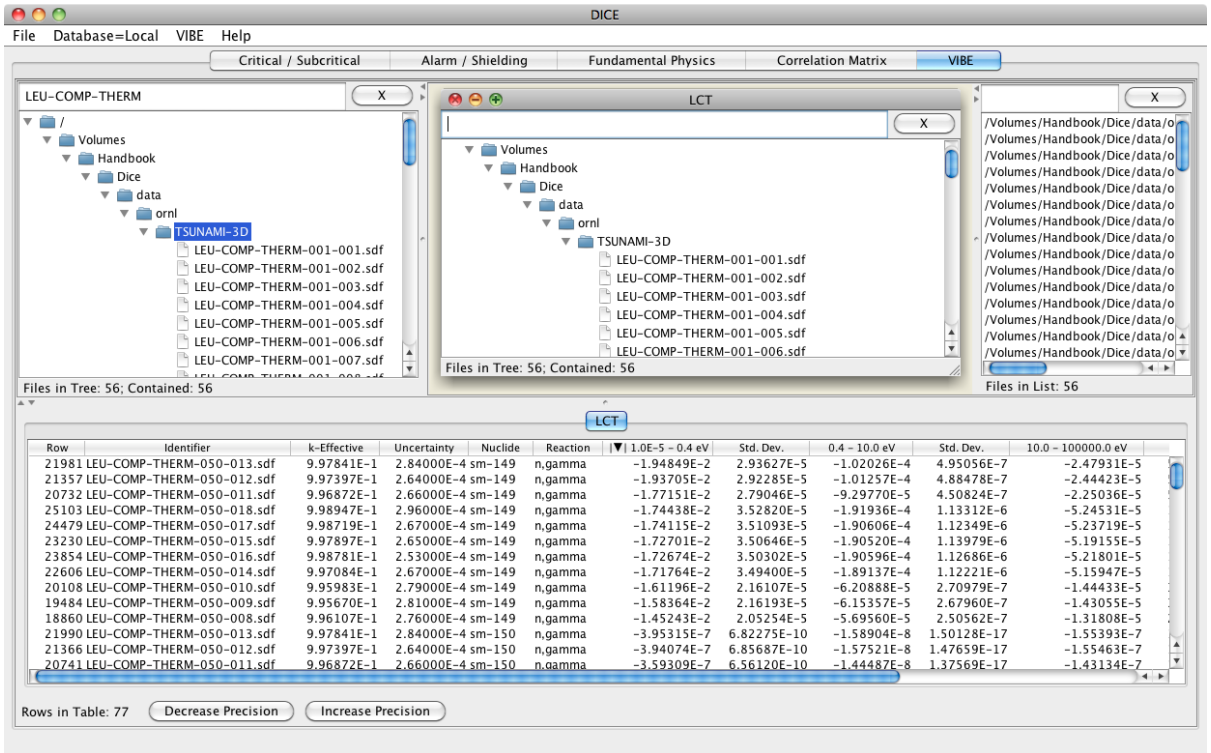

Figure 2. Use of VIBE to identify experiments with the largest sensitivity to ^{149}Sm (n,gamma) at thermal energies.

Additionally, the normal DICE interface can be used to visualize sensitivity data for available experiments, even without loading the VIBE plug-in version, as shown in Figure 3.

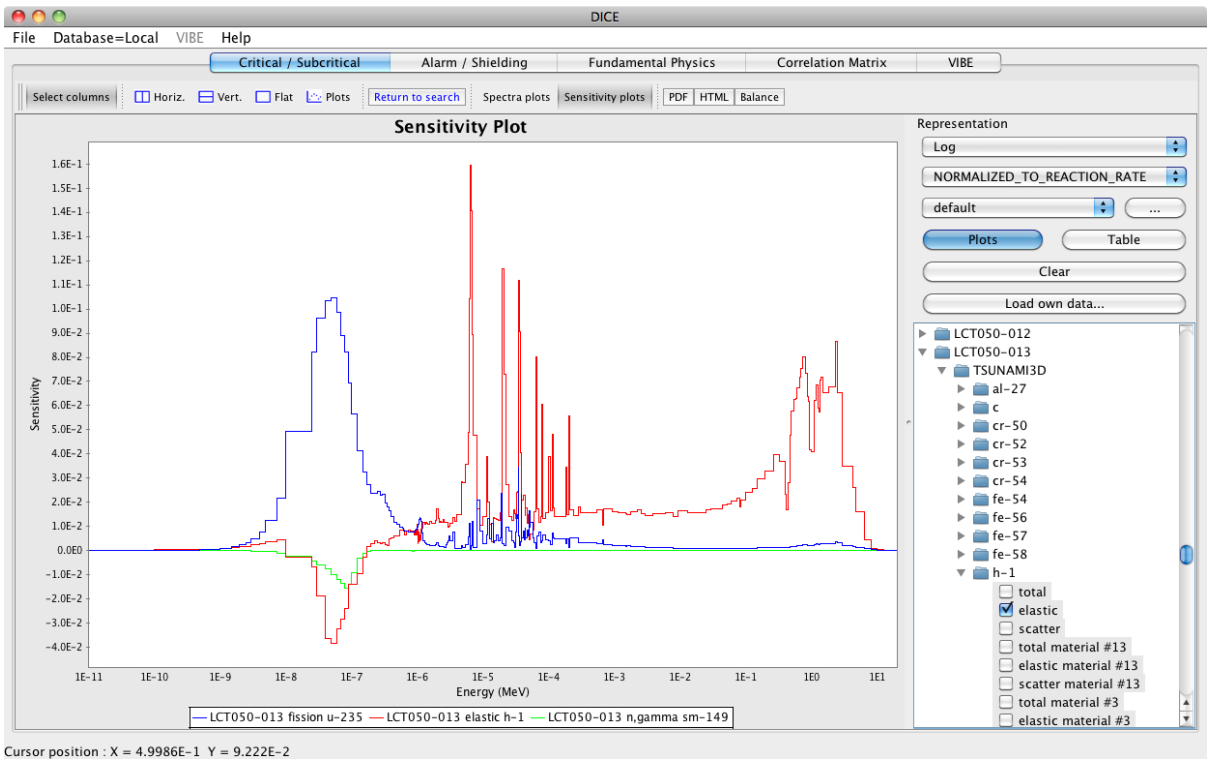

Figure 3. DICE plot of TSUNAMI sensitivity data.

6 CONCLUSIONS

With hundreds of SDF files available with the 2010 distribution of the IHECSBE, criticality safety practitioners can more readily apply the advanced validation techniques of TSUNAMI in their work. The availability of numerous SDFs also facilitates the identification of gaps in available benchmarks that need to be addressed with experiments through the C_EdT process. ORNL will continue to develop additional benchmark models and SDF files for distribution through the IHECSBE, with continued support from the DOE NCSP. It is hoped that in the coming years every benchmark in the IHECSBE will have a corresponding quality Scale input and SDF file available.

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