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INTRODUCTION

The ***T***ools for ***S***ensitivity and ***UN***certainty ***A***nalysis ***M***ethodology ***I***mplementation (TSUNAMI) codes were first released with SCALE 5 in June of 2004.[1] Since that time, ongoing research at Oak Ridge National Laboratory (ORNL) has led to a number of enhancements in previously released codes and the development of additional software tools that further enhance the capabilities of SCALE and TSUNAMI. The capabilities described in this paper are expected to be released with SCALE 5.1.

ENHANCEMENTS TO SCALE 5 CODES AND DATA

Implicit Sensitivity Coefficient Generation

One obstacle to many TSUNAMI analyses is the limit of 50 nuclides with resolved-resonance data in a system model imposed by the NITAWLST code. NITAWLST produces resonance self-shielded cross sections and their sensitivities to input data, the so-called implicit sensitivity.[2] The 50-nuclide limitation was partially imposed by limitations in the GRESS [3] software used for automatic differentiation in NITAWLST. An updated version of GRESS has been developed that increases the previous number of allowed independent parameters from 200 to 10,000. Additionally, the updated GRESS provides for automatic differentiation of a subset of Fortran 90 source code, whereas the implementation of GRESS used with SCALE 5 would process only Fortran 77.

An updated NITAWLST code developed with the new version of GRESS has no limit on the number of nuclides in the system model. Additionally, an updated BONAMIST code, used for producing resonance self-shielded cross sections and their sensitivities to input data for the unresolved-resonance region, has been developed with the new version of GRESS. Although less restrictive than NITAWLST, the SCALE 5 version of BONAMIST limited the analysts to a sum of nuclides and mixtures not exceeding 200. The updated BONAMIST increases this limit to a sum of nuclides and mixtures in a single unit cell not exceeding 10,000.

Expanded Cross-Section Covariance Data

Much of the sensitivity and uncertainty (S/U) analysis in TSUNAMI requires utilization of nuclear data uncertainties. The initial release of SCALE 5 included covariance libraries containing uncertainty data generated mainly from ENDF/B-V. Because SCALE 5.1 will include multigroup libraries based on ENDF/B-VI,[4] it was necessary to create new covariance data as well. Furthermore, only a limited amount of nuclear data uncertainty information is available in both ENDF/B-V and VI. Therefore, SCALE 5.1 provides approximate values for much of the missing uncertainty data by utilizing experimental uncertainties in integral measurements of thermal cross-section and resonance integrals. A statistical method based on random sampling of resonance parameter data has also been developed. The covariance library in SCALE 5.1 is more complete and is applicable to a wider range of applications than the previous libraries.

NEW CAPABILITIES FOR SCALE 5.1

Implicit Sensitivity Coefficient Generation with CENTRMST

A significant addition to SCALE 5.1 is the ENDF/B-VI cross-section data library. However, the NITAWLST code is capable of processing data only in the ENDF/B-IV or ENDF/B-V formats. The CENTRM code, initially released with SCALE 5, uses one-dimensional deterministic neutron transport to produce a flux solution based on point-wise cross-section data. The point-wise solution can be used to produce problem-dependent resonance self-shielded cross sections for the resolved-resonance region in multigroup format.

The updated version of GRESS was used to produce differentiated versions of CENTRM and its associated data-processing code PMC. The sensitivity versions of these codes are called CENTRMST and PMCST and process point-wise data from ENDF/B-V and ENDF/B-VI into problem-dependent multigroup cross sections and produce the sensitivity of the multigroup cross sections to data input to their calculation. This sensitivity information is used to produce the implicit portion of the sensitivity coefficients in the SAMS module of SCALE.

Data Adjustment Capabilities with TSURFER

A generalized linear least-squares computational tool called TSURFER ("***T***ool for ***S/U***-analysis of ***R***esponse ***F***unctionals using ***E***xperimental ***R***esults") combines computed and measured benchmark results and provides an estimate for the computational bias and uncertainty. TSURFER minimizes the overall discrepancy (chi squared) between a selected set of measured and calculated responses such as k_{eff} by adjusting the nuclear data and experimental parameters in a manner consistent with their uncertainties. The least-squares minimization procedure may also be used to adjust the calculated values of one or more "application responses" for which experimental results are not available. The original set of benchmark measurements may be filtered based on similarity coefficients compared with the application system to ensure that an appropriate set of experiments is used to validate the calculation of the application response.

For example, the application system could correspond to a proposed arrangement of fissile materials in a criticality safety study. The nuclear data adjustments that minimize differences in the computed and measured k_{eff} values for the selected set of benchmark criticals will also indirectly adjust the calculated multiplication factor of the application system, since the same nuclear data are used. The difference between the adjusted and the original k_{eff} value of the application system corresponds to the predicted bias in the initial calculation. The adjustment methodology also provides the prior and adjusted uncertainties in the application response. Thus, the TSURFER code provides a rigorous approach to incorporate benchmark measurements into the overall criticality safety analysis, providing an estimate for the computational bias and uncertainty in a consistent manner.

RESULTS

Data Library and Implicit Sensitivity Coefficients

Results of a series of calculations using various data libraries and resonance self-shielding codes to analyze a single sample problem are presented in this section. The sample problem is based on an unreflected rectangular parallelepiped consisting of a homogeneous mixture of UF_4 and paraffin with an enrichment of 2% in ^{235}U. The $H/^{235}U$ atomic ratio is 293.9:1. The dimensions of the experiment were 56.22 × 56.22 × 122.47 cm.[5] The experiment was modeled as a sphere with a critical radius of 38.50 cm.

The TSUNAMI-1D sequence was used to assess the consistency of different resonance self-shielding codes and cross-section data libraries in sensitivity coefficient generation. First, this problem was analyzed with the SCALE 238-group ENDF/B-V multigroup library using the SCALE 5 versions of BONAMIST and NITAWLST and the enhanced versions of BONAMIST and NITAWLST developed for SCALE 5.1. Next, the same problem was analyzed in the 238-group structure with ENDF/B-V and ENDF/B-VI libraries using the SCALE 5 version of BONAMIST for processing unresolved resonances and CENTRMST/PMCST to process the resolved resonance data. Table I shows the energy-integrated sensitivity of k_{eff} to the total cross section of each nuclide in the model. The results are displayed as the implicit sensitivity, which is generated using the sensitivity data from the resonance self-shielding codes, and the complete sensitivity, which represents the true sensitivity of k_{eff} to the particular cross section and is the sum of the explicit and implicit components, where the explicit component is the sensitivity of k_{eff} to the problem-dependent cross-section data.

The results agree quite well across all data libraries and codes. The SCALE 5 and SCALE 5.1 versions of BONAMIST and NITAWLST produce exact agreement using the ENDF/B-V library. The CENTRMST calculation with the ENDF/B-V library produces exact agreement with the other ENDF/B-V results for the complete sensitivity, with only minor differences for the implicit sensitivity. The CENTRMST results using the ENDF/B-VI library present small variations from the ENDF/B-V results, but some differences are expected with the new library.

CONCLUSIONS

The enhanced and additional TSUNAMI capabilities for SCALE 5.1 provide a number of advantages over the SCALE 5 implementation. The improved capabilities include analysis of models with more than 50 nuclides with resolved resonance data, assessment of uncertainty with an improved cross-section covariance data library, processing of ENDF/B-V and VI data with CENTRMST, and estimation of biases and uncertainties with TSURFER.

TABLE I. Implicit and Complete Sensitivity Coefficients for Total Cross Sections with Differing Resonance Self Shielding Codes and Data Libraries.

Isotope	SCALE 5 NITAWLST ENDF/B-V k_{eff} = 1.0026		SCALE 5.1 NITAWLST ENDF/B-V k_{eff} = 1.0026		SCALE 5.1 CENTRMST ENDF/B-V k_{eff} = 1.0031		SCALE 5.1 CENTRMST ENDF/B-VI k_{eff} = 1.0025	
	Implicit	Complete	Implicit	Complete	Implicit	Complete	Implicit	Complete
^{1}H	-3.08E-02	2.26E-01	-3.08E-02	2.26E-01	-3.08E-02	2.26E-01	-3.10E-02	2.24E-01
^{12}C	-3.49E-02	2.49E-02	-3.49E-02	2.49E-02	-3.46E-02	2.49E-02	-3.50E-02	2.47E-02
^{19}F	-4.00E-03	3.90E-02	-4.00E-03	3.90E-02	-4.00E-03	3.90E-02	-3.74E-03	4.00E-02
^{235}U	-1.20E-04	2.52E-01	-1.20E-04	2.52E-01	-1.91E-04	2.52E-01	-1.79E-04	2.53E-01
^{238}U	3.84E-02	-2.08E-01	3.84E-02	-2.08E-01	3.85E-02	-2.08E-01	3.85E-02	-2.06E-01

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