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LETTER REPORT

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1. INTRODUCTION

The objective of the NCSP Analytical Methods program element is to sustain state-of-the-art radiation transport modeling capabilities and the expertise necessary to develop, maintain, and disseminate the analytical tools and data libraries in a manner that is responsive to the needs of those responsible for developing, implementing, and maintaining criticality safety. To this end, the objective of the AMPX[1] Development and Maintenance Subtask is to ensure that the AMPX cross-section processing system is available to prepare cross-section and covariance libraries that are needed by SCALE[2] and other radiation transport packages to support criticality safety analyses of systems with fissionable material. Moreover, the task ensures that the cross-section processing software is current and up-to-date with the Evaluated Nuclear Data File (ENDF/B)[3] formats and procedures for disseminating evaluated cross-section data provided through new measurement and evaluation work efforts. The AMPX subtask provides for the production of data libraries needed for criticality safety analyses. As such, the task provides the "bridge" between the nuclear data evaluations and the radiation transport software. In the absence of the AMPX cross-section processing task, the ability to maintain and update the SCALE nuclear data libraries (cross-section and covariance data) would be hindered. Therefore, the AMPX Development and Maintenance Subtask ensures that SCALE is up-to-date with the latest cross-section data for supporting criticality safety analyses. This letter report provides a summary of the FY 2011 AMPX development and maintenance activities that have been performed in support of the NCSP. Specifically, the report summarizes the AMPX code system updates that have been made to the software package and documents the cross-section library updates that have been made for the SCALE radiation transport package. In addition, the report documents testing activities that have been performed to process available cross-section and covariance data files to ensure the latest ENDF/B data files can be processed properly.

2. AMPX CODE SYSTEM UPDATES

2.1 PUFF-IV Update Related to LRF=7

In November 2009, the U.S. ENDF/B Cross Section Evaluation Working Group (CSEWG) approved a format extension to provide a space for the scattering radius uncertainty in the resonance parameter covariance formats. The PUFF-IV module uses the SAMMY/SAMRML library[4] to calculate the sensitivities of the cross section to the resonance parameters. This change has been previously incorporated into PUFF-IV and the calculation of the radius uncertainty was tested. Most evaluations in ENDF/B-VII Release 1 use Single-level or Multi-level Breit-Wigner (LRF=1 and LRF=2) or Reich-Moore (LRF=3) formats. Some newer evaluations are now using the new R-Matrix Limited format (LRF=7), which allows a variable number of open channels per spin group. The updated PUFF-IV module and SAMRML library worked without a problem for evaluations using LRF=7 with a constant number of channels per spin group but failed if the number of open channels depends on the spin group. In the pre-release ENDF/VII.1 there are only two evaluations, ^{35}CL and ^{19}F that use LRF=7. Of the two evaluations, only ^{19}F has different numbers of open channels per spin group. Thus, PUFF-IV gave wrong results for ^{19}F, although the evaluation does not give uncertainties on the radius. The error was traced to a bookkeeping error in SAMRML and was corrected. The results obtained by SAMMY and PUFF-IV for ^{19}F were compared and showed good agreement with one another. A test case exercising the above feature was added to the test suite of PUFF-IV.

2.2 Updates for SCALE Resonance Self-shielding Capabilities

The multi-group (MG) libraries distributed with SCALE 6.1 contain Bondarenko self-shielding factors based on the narrow-resonance approximation. The factors, which give the ratio between self-shielded and infinite dilute cross sections, are tabulated at a number of predefined background cross sections and temperatures. During a transport calculation, the correct self-shielded cross section is determined by

interpolating between the predefined background and temperature values. It was desired to add intermediate resonance (IR) factors, based on the intermediate resonance approximation. The effective shielded cross section in a resonance group g can be written as:

$$\sigma_{x,g} = \frac{\int_{\Delta u_g} \sigma_x(u)\phi(u)du}{\int_{\Delta u_g} \phi(u)du} .$$

In the narrow resonance approach, the neutron spectrum is simply inversely proportional to the total cross section:

$$\phi(u) = \frac{const.}{\sigma_t(u)} .$$

In a more sophisticated IR method, the flux spectrum can be written as:

$$\phi(u) = \frac{\sigma_b}{\sigma_a(u) + \sigma_b} ,$$

where a background cross section is defined as:

$$\sigma_b = \frac{1}{N_R} \sum_{i=all} N_i \lambda_i \sigma_{p,i} .$$

N_R is the atomic number density of the resonance nuclide, N_i is the atomic number density of the isotope i and λ_i is the IR parameter for the isotope and $\sigma_{p,i}$ is the potential cross section of isotope i.

In order to determine background cross sections, CENTRM/PMC calculations are run to determine the self-shielded cross section for a set of homogenous mixtures. The number density of a background material (for example water or graphite) is varied to generate different values for the background cross section. A similar procedure is followed to calculate the λ_i values. Two new modules (LAMBDA and IRFFACTOR) have been added to AMPX to calculate the λ_i and the IR factors. The modules automatically run CENTRM/PMC sequences at varying number densities of the background isotope. The number density is varied until background values over the entire desired range can be interpolated within a user-specified precision. From these calculations, the λ_i and the IR factors are determined and saved in the library. Libraries containing λ_i and the IR factors have been generated for the 238-group general purpose cross-section library and the 81-group broad-group library. Code changes in SCALE 6.1 are needed to use the updated libraries. The libraries and the corresponding code changes in SCALE are currently undergoing final testing.

2.3 PLATINUM Improvements

Many of the actions that are performed by various AMPX modules have been placed in functions that can be utilized by all modules. These functions deal with 1-D continuous-energy (CE) or point-wise data as well as the kinematics data and are utilized by both CE and MG library generating routines. The PLATINUM module had its own custom implementation of reading 1-D point data, which necessitated the use of numerous scratch files. The coding in PLATINUM has been updated to take advantage of the 1-D library function. This update removed the need for scratch files. Similarly, since the mass ratio update for all SCALE libraries (see section 3.3) necessitated the development of a new module to read

and write CE libraries, the functions from the new module are now used in PLATINUM as well. The same structures for CE kinematics data are now used throughout the AMPX code system. These improvements make the flow in PLATINUM clearer and will allow for easier maintenance and future updates to support new formats.

3. NUCLEAR DATA LIBRARY UPDATES

3.1 Prototypic JENDL-4 MG Library

In order to test processing with the AMPX code system, Japanese Evaluated Library (JENDL-4)[5] data files have been downloaded and processed into a MG library. On occasion, the JENDL-4 files use the ENDF6 format in a subtle different way than the ENDF/B data files. These differences can uncover overstepped bounds and improperly allocated arrays in the code. Processing of the JENDL-4 files did uncover some overstepped bounds in the MG processing, and the error has been corrected. A prototypical MG library based on JENDL-4 has been generated.

Likewise, while processing the JENDL-4 graphite evaluation into a CE library for benchmark testing, an overstepped bound was discovered. For CE cross-section files all temperature dependent reactions are unionized into a common energy grid. In order to keep the grid size manageable, points that are closer than some specified difference are not added. The two routines that handle the energy mesh creation used a slightly different criterion (less than instead of less than or equal) to check for point differences. This difference could lead to overstepped bounds or to a zero cross section calculated on the union mesh. Both of these cases have been addressed and graphite can now be processed into MG and CE libraries using the current AMPX code package.

3.2 Processing ENDF/B-VII.1 Beta 3 Covariance Evaluations

The pre-release ENDF/B-VII.1 database contains covariance information for many more nuclides than ENDF/B-VII.0. In comparison, the covariance library distributed with SCALE 6.1 attempts to cover all nuclides in the available criticality libraries. Where high-fidelity covariance data are not available, low-fidelity covariance data are used in the SCALE library. Because the ENDF/B-VII.1 library will have more high-fidelity evaluated covariance data, there is a need to update the SCALE covariance data information for criticality safety analyses. In order to assess the ability for AMPX to be used to process the new ENDF/B-VII.1 covariance data, AMPX has been used to process the pre-release ENDF/B-VII.1 data and demonstrate the functionality of the covariance libraries with SCALE. In FY 2012, the ENDF/B-VII.1 database should be released from the National Nuclear Data Center (NNDC), and ORNL will begin work to prepare production-level cross-section and covariance data libraries for SCALE to support nuclear criticality safety applications.

The SCALE covariance library contains 44 neutron energy groups. When the current SCALE library was created, cross-section data were passed to PUFF-IV in the form of a 44-group AMPX master cross-section library, which is collapsed from the 238-group library using a LWR flux spectrum. At that time, this was the only way to pass cross-section data to PUFF-IV. With recent modifications, point-wise cross-section data are also allowed. In order to assess the impact of the new ENDF/B-VII.1 Beta 3 covariance information on benchmark calculations, all ENDF/B-VII.1 Beta 3 data have been processed with PUFF-IV using both methods to pass the cross-section information. Differences between the two methods have been discussed in the FY 2010 AMPX annual report and in an ANS paper.[6] For materials that do not have covariance information in ENDF/B-VII.1 Beta 3, the covariance matrices from the current SCALE library were used.

Benchmark cases using TSUNAMI were run using the new covariance library (ENDF/B-VII Beta 3) and the results were compared with the old values (SCALE 6.1). As an example the change in c_k, the correlation coefficient, which represents the degree of correlation in the uncertainties between the two systems, is shown in **Figure 1**. The cross-section uncertainties calculated from ENDF/B-VII.1 Beta 3 can be higher [for example ^{1}H elastic and (n,γ)] or lower [for example ^{151}Sm (n,γ)]. In addition, some of the $\bar{\nu}$ uncertainties, which generally have a large effect on the uncertainty in k_{eff}, have also been updated with the new evaluations.

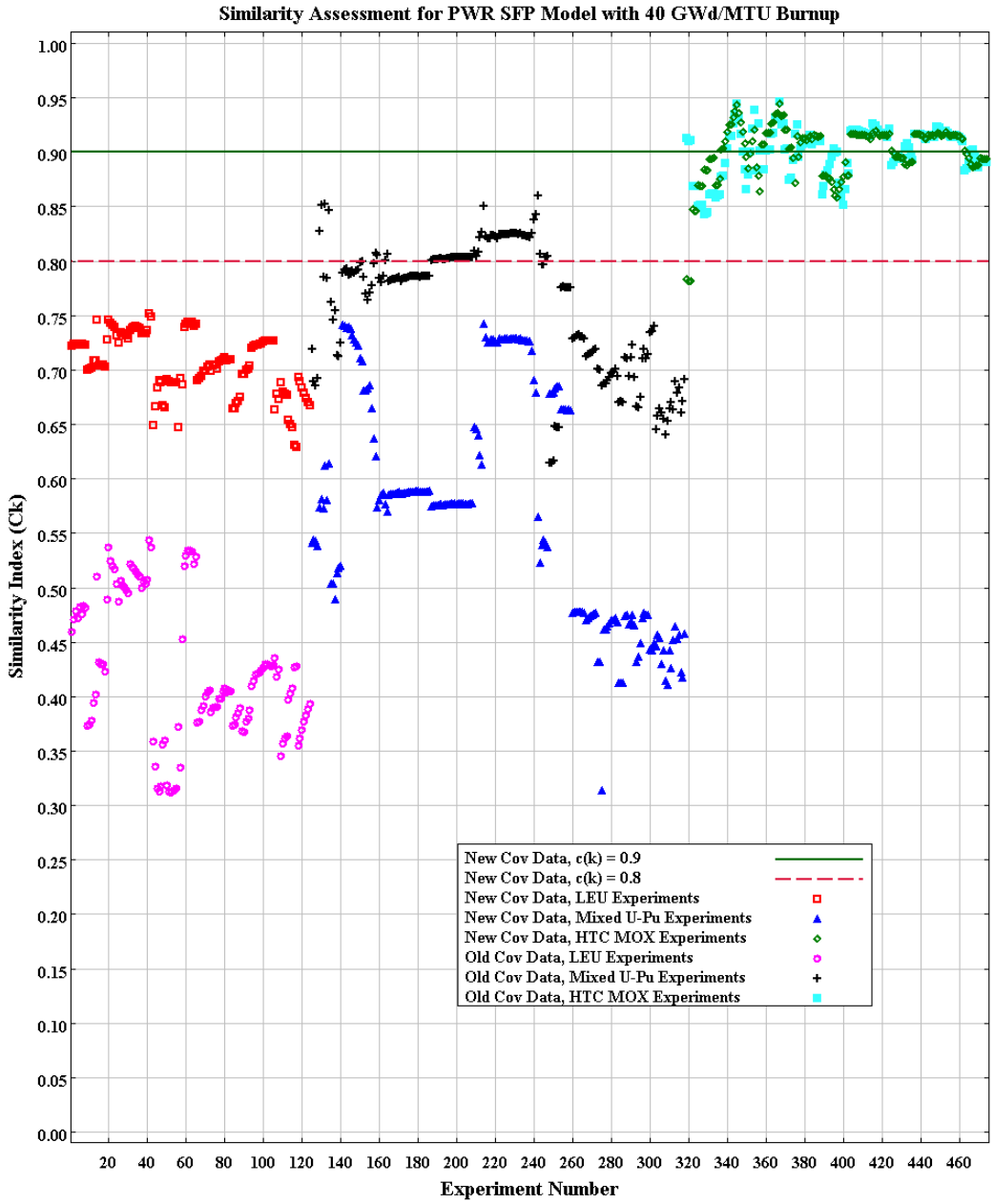

Figure 1: Plot showing change in c_k due to changed covariance data.

3.3 SCALE 6.1 Library Updates

The MG and CE libraries distributed with SCALE 6.1 contain the mass ratio from the ENDF cross-section evaluation file. The mass ratio stored in the libraries is taken directly from the ENDF file and is

used in SCALE to calculate mixing tables. However, SCALE also uses the mass ratio given in the Standard Composition library and the two values are not always in agreement. Recently, the Standard Composition Library in SCALE 6.1 was updated to use the atomic mass evaluations by A.H. Wapstra, G. Audi, and C. Thibault.[7,8] In order to be consistent, the mass ratios in the AMPX-generated cross-section libraries were also updated. In the case of MG libraries, a suitable module that reads and writes MG libraries already existed, around which a wrapper program was written to update the mass ratio. A module that reads and writes CE libraries did not exist and needed to be created in order to change the mass ratios in the CE libraries. All MG and CE libraries based on ENDF/VII.0 and ENDF/VI.8 were updated to use consistent mass ratio values. Numerous test cases and benchmarks were run and compared with previous results before the updated libraries were distributed with SCALE 6.1. After the release of SCALE 6.1, the SCALE development team started to use different ID values for metastable nuclides and thermal moderators. In the case of the CE and MG libraries, this merely meant a change of ID and the file name in the case of the CE libraries.

With regard to depletion capabilities, the current AMPX procedure to create ORIGEN depletion libraries does not work on evaluations that contain resonance parameters in ENDF/B File 2. This is the case for many of the ENDF/B-VII.0 evaluations. For the library used with the ORIGEN depletion code, we took the opportunity to change the processing slightly to accommodate ENDF/B-VII.0 data. Our objective was to use ENDF/B-VII.0 evaluations for the new ORIGEN libraries, in order to be consistent with the data used in the criticality libraries. The new procedure uses the same point-wise data as generated for the SCALE criticality libraries and produces additional point data from the branching information in ENDF/B File 9 and File 10. The point-wise data are produced using POLIDENT. The module LIPTON, which previously combined ENDF/B File 3 (point-wise cross section data) and Files 9 and 10 data, was changed to use the data generated by POLIDENT. Unfortunately, the ENDF/B-VII.0 evaluations did not have sufficient File 9 and File 10 data to make an ORIGEN cross-section library as complete as the current library. Therefore, we continued to use the Joint Evaluated Fission and Fusion (JEFF-3.0/A) evaluated data. However, the capture cross-section data for ^{239}Np were taken from ENDF/B-VII.0 as JEFF-3.0/A did not give good results in ORIGEN. In addition, the branching ratio for ^{241}Am capture data was also taken from ENDF/B-VII.0.

ORIGEN uses a gamma library describing the gamma energies and intensities emitted after decay. The current gamma library is based on older versions of Evaluated Nuclear Structure Data Files (ENSDF), ENDF and JEFF. An updated library based on the NuDat library,[9] which is based on the newest ENSDF data, has been prepared. NuDat provides X-ray and gamma data for beta+, beta-/EC and alpha decay from metastable isotopes down to the daughter ground state in addition to decay gamma and x-rays from metastable state to ground state. Thus, the same gamma or x-ray transition can be given twice, once from the decay of the parent to the metastable state of the daughter down to the ground state and once for the decay of the daughter itself. An example is ^{137}Cs, which decays via beta to metastable ^{137}Ba, which emits a 661.657 keV gamma line during the decay to the ground state. NuDat gives this line for the decay of ^{137}Cs as well as for ^{137}Ba. The ORIGEN library can contain this line only once, namely for ^{137}Ba. While this case is relatively simple, there are other cases where the same line appears in the library for the daughter as well as the parent, but with a different intensity than given in NuDat to account for branching. A new AMPX module, GNUDAT, was added that parses the NuDat data, calculates the correct intensities for the ORIGEN gamma library and writes out a new gamma library. Since NuDat contains inconsistencies, the program tries to flag these and present them to the user for review. A new ORIGEN gamma library for use in SCALE 6.1 was prepared.

The shielding libraries distributed with SCALE contain dose functions for neutrons and gammas. While converting the gamma dose functions for use in CE-MONACO, which is a new continuous-energy fixed source transport code in SCALE, it was discovered that ANSI-1991 gamma dose function values were too high. The AMPX module JERGENS, which is used for generating the dose functions, was corrected and

the SCALE MG libraries were updated. A SCALE Data Revision Report (DRR) was prepared, and the updated libraries were moved into the production version of SCALE and released in SCALE 6.1.

4. TESTING NEW CROSS-SECTION EVALUATIONS FOR CONFORMANCE TO ENDF/B FORMATS AND PROCESSING CAPABILITIES

Complete new evaluations in the resolved resonance region have been developed under the ORNL NCSP Nuclear Data Program Element for ^{50}Cr and ^{54}Cr. The evaluations include ENDF/B File 2 (resolved resonance parameters) as well as File 32 (resolved resonance parameters for covariance information). High-energy data were provided by P. Pereslavtsev, A. Konobeyev, L. Leal, and U. Fischer from KIT, Karlsruhe Germany. In addition, S(α,β) data for SiO_2 were produced. This evaluation was produced in collaboration with North Carolina State University (NCSU) in November 2010 using a modified LEAPR code. Modifications were made to accommodate coherent elastic scattering in the SiO_2 alpha quartz crystal structure. The evaluation is performed for the entire SiO_2 molecule and is normalized to natural silicon, with oxygen being treated as a zero-scatterer. The phonon frequency distributions for natural silicon and ^{16}O in SiO_2 were produced by the VASP and PHONON codes using DFT methodology.[10] Note that alpha quartz transitions to beta quartz at 846 K. Both phases may be viewed on a hexagonal lattice. However, alpha quartz has trigonal symmetry while beta quartz has hexagonal symmetry. The ENDF/B formatted files for the noted evaluations were processed through the AMPX code system, generating MG and CE libraries as well as covariance libraries to ensure that the files could be processed correctly and give the expected results. After successful processing with AMPX, the ORNL-evaluated data files were submitted to NNDC.

5. LIST OF PUBLICATIONS

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6. SUMMARY

During FY 2011, the AMPX software has been updated to improve the computational performance of the cross-section processing package mainly with respect to the CE library generation. Efforts are currently under way to finalize the AMPX users manual, and the code package will be released from RSICC in FY 2012. In addition, AMPX has been used to test new ORNL cross-section evaluations submitted to NNDC. Furthermore, AMPX has been used to update or regenerate the SCALE CE and MG cross-section libraries that are needed by the criticality safety community. The updated cross-section libraries have been distributed with SCALE 6.1.

7. REFERENCES

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