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1. INTRODUCTION

The objective of the Nuclear Criticality Safety Program (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 2015 AMPX development and maintenance activities that have been performed in support of the NCSP. Specifically, the report summarizes the AMPX code system updates and modernization accomplishments that have been made to the software package. Also, the report 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. This report satisfies the following reporting milestone in the NCSP FY16-20 Five Year Plan:

- Document AMPX modernization and technical support for SCALE continuous energy (CE), multigroup (MG), and covariance libraries and report status annually to the NCSP Manager (AM3: Q2)

2. AMPX CODE MODERNIZATION

2.1 INTERACTION WITH ENDF

As reported in the previous NCSP AMPX annual report,[4] the module Y12, used to generate Collision Kinematics Data Files, was modernized. The modernization added a layer between reading the ENDF data and processing the data. This should allow the use of the new GND format[5] for ENDF data with a change in the ENDF reading functions only and not the processing part itself. Previously this layer only processed kinematic data. The layer has been extended to include resonance parameters for the resolved range (RR) as well as the unresolved range (URR) along with resonance covariance information, contained in File 2 and File 32. New classes have been added that read the resonance information from the ENDF file and store them in memory in resonance structures. In addition, development of an API for calculating cross section data has been started. The API provides functions independent from the resonance formalism used. Codes that need cross section or derivatives at a given energy will use the API and therefore be independent of the resonance formalism used in the ENDF format. Prototypical implementations for the API using the implementation used in SAMMY[6] and the PUFF covariance processing module have been implemented to test the API. No rigorous unit tests have yet been added for the implementation as they will be tested and used in future modernization efforts.

2.2 MODERNIZATION OF X10

The module X10 is used to generate the cross section data and the scattering matrices in MG format by group averaging the point-wise data. The module has been modernized to take advantage of new integration routines and the more modular approach to access MG data.

The group averaged 1-D cross section is given by:

$$\frac{1}{\int_{E_1}^{E_2}\varphi(E)dE}\int_{E_1}^{E_2}\sigma(E)y(E)\varphi(E)\,dE \tag{1}$$

where $\sigma(E)$ is the point-wise cross section and $\varphi(E)$ is the flux. The yield $y(E)$ is only different from 1 if fission yields are calculated. This integral can be solved numerically if the distributions use linear interpolation. A new C++ class was added to calculate this integral.

Scattering matrices are calculated for a given incident energy group and exit energy group, and they are always in Legendre moments. Assuming the incident energy group i has boundaries $\lfloor E_1, E_2\rfloor$ and the exit energy group j has boundaries $\lfloor {E'}_1, {E'}_2\rfloor$, the scattering matrix element at $[i,j]$ for Legendre moment l is calculated as:

$$\frac{1}{\int_{E_1}^{E_2}\varphi(E)dE}\int_{E_1}^{E_2}dE y(E)\sigma(E)\varphi(E)\int_{{E'}_1}^{{E'}_2} f_l\,(E,E')dE', \tag{2}$$

where $f_l(E,E')$ is the exit energy distribution at incident energy E for the lth Legendre order and all other parameters are as before. The inner integral at a given energy E_m is calculated using unit-based interpolation[6]. Assume the desired incident energy E_m lies between two incident energies present in the distribution— $f_l(E_1,E')$ and $f_l(E_2,E')$ —where $f_l(E_1,E')$ extends from ${E'}_1^{low}$ to ${E'}_1^{high}$, and $f_l(E_2,E')$ extends from ${E'}_2^{low}$ to ${E'}_2^{high}$. From this the lower boundary at E_m is calculated as

$${E'}_m^{low} = {E'}_1^{low} + \frac{E_m-E_1}{E_2-E_1}\left[{E'}_2^{low} - {E'}_1^{low}\right], \tag{3}$$

and upper boundary as:

$${E'}_m^{high} = {E'}_1^{high} + \frac{E_m-E_1}{E_2-E_1}\left[{E'}_2^{high} - {E'}_1^{high}\right]. \tag{4}$$

The energy bound ${E'}_m^b$ in the exit energy distribution at E_m is translated to an energy bound in the first exit energy distribution as:

$${E'}_1^b = {E'}_1^{low} + \frac{{E'}_m^b - {E'}_m^{low}}{{E'}_m^{high} - {E'}_m^{low}}\left[{E'}_1^{high} - {E'}_1^{low}\right]. \tag{5}$$

and correspondingly for the upper exit energy distribution. Since the exit energy distribution for a given incident energy and l is just a linear function of exit energy, we can calculate the inner integral for each of the two bounding exit energy distributions analytically using the updated integral bounds. To get the value of the integral at E_m, we linearly interpolate between the integrals calculated for the two bounding distributions.

The outer integral is performed for all Legendre orders at the same time using a fourth order Runge-Kutta method with adaptive step size[7], except when the angular distribution is discrete and the integral can be calculated analytically. A C++ class has been added that can calculate these integrals.

For most reactions the exit energy is smaller or equal to the incident energy. If the exit energy in the two bounding distributions is smaller or equal to the incident energy, we ensure that the same is true in the interpolated panel. Due to numerical instabilities the interpolated exit energy range can be slightly larger than the incident, usually for small incident energies. On the other hand, in the thermal range there can be substantial up-scatter for free gas scattering or thermal moderators. In order to preserve the correct behavior in the interpolated panel, two unit based regions are used, one extending from low exit energy to incident energy, the other from incident energy to the high exit energy. Fission reactions also usually have exit energy spectra that extend below and above the incident energy and interpolation needs to be done with one unit based region over the entire exit energy range to preserve the spectrum. The module X10 selects the correct interpolation behavior based on the reaction ID of the scattering matrix. Selecting the correct unit based approach has become more important for free-gas scattering as the module Y12 now generates point-wise scattering data for free-gas scattering. Previously the MG free-gas scattering data were produced using the module FLANGE, which generated MG scattering matrices in the thermal range. While the calculation is very efficient, it becomes numerically unstable for $l > 3$. Using the point-wise free-gas scattering, while much slower, has no such limitations.

Collapsing the group averaged scattering matrix for $l = 0$ should give the same value as the group averaged cross section data. As the group averaged cross section is integrated analytically, it is assumed to be the more precise value of the two. Therefore, the scattering matrix for all values of l is normalized so that the $l = 0$ matrix collapses to the desired 1-D cross section data.

In addition, X10 now offers the possibility to use a flux library that contains ZA and temperature dependent weighting spectra. The correct flux will then be retrieved from the library before doing the group averaging. This gives the user a higher flexibility in selecting the weighting spectrum, and the MG libraries distributed with SCALE 6.2 do use ZA and temperature dependent flux spectra.

Since MG library data are now in memory, it is much easier to manipulate the data. Therefore, we added a new C++ class (MgCorrect) that can correct data before saving the final library. The class can correct the MG library as follows:

- 1-D cross section values below a user-specified value are set to 0. This includes negative cross section values.

- For thermal moderators like ^{1}H in H_2O, the elastic cross section (MT=2) is set to the 1-D collapse of the thermal scattering matrices in the thermal range. The first thermal group defines the extent of the thermal range. If the evaluation uses the free-gas approximation for the thermal scattering matrices, the thermal scattering matrices are renormalized such that when collapsed they result in the elastic cross section as calculated from the ENDF information.

- The elastic scattering matrix (MT=2) is set to zero in the thermal range, where the first thermal group again defines the thermal range. The assumption is that the free gas scattering matrix should be used in this range.

- An AMPX master library should only contain up-scatter in the thermal range. Thus, scattering matrices are corrected to not contain any up-scatter terms outside the thermal range. Any up-scatter terms are added to the diagonal matrix element.

- All redundant 1-D cross section values are recalculated from the partial cross section values.

- If the library contains gamma production information, the module checks whether all production matrices are given relative to the cross section. If not, the relevant scattering matrices are renormalized to be relative to the cross section.

- If a scattering matrix has a $(P_l, l > 0)$ term that is non-zero and the P_0 term is zero, then the $(P_l, l > 0)$ is also set to zero.

- If the exit energy distribution for delayed and prompt fission is given, the total χ-distribution is recalculated.

The module SIMONIZE that generates the final MG data by combining the results from X10 and the FABULOUS, has also been modernized to take advantage of the in-memory MG library resource. In addition, it uses MgCorrect to produce a final polished library.

2.3 MODERNIZATION OF FABULOUS

The module FABULOUS computes data needed for resonance self-shielding of MG cross sections with the Bondarenko method[9]. The Bondarenko method represents self-shielded cross sections in terms of temperature and a background cross section parameter σ_0 which indicates the degree of self-shielding:

$$s_{x,g}^{(j)}(s_0,T) = \frac{\int_g s_x^{(j)}(E,T) j\,(E,s_0,T)\,\mathrm{dE}}{\int_g j\,(E,s_0,T)\,\mathrm{dE}}, \tag{6}$$

where $\sigma_{x,g}^{(j)}(\sigma_0,T)$ is the self-shielded MG cross section in group g for reaction type x and nuclide j, corresponding to background cross section σ_0 and temperature T. The weighting function $\varphi(E,\sigma_0,T)$ approximates the fine-structure flux spectrum for a mixture containing resonance nuclide j at varying dilutions as defined by the value of σ_0. Bondarenko shielding factors, also known as f-factors, are computed from the expression

$$f_{x,g}^{(j)}(\sigma_0,T) = \frac{\sigma_{x,g}^{(j)}(\sigma_0,T)}{\sigma_{x,g}^{(j)}(\varphi_{ref},T_{ref})}, \tag{7}$$

where the denominator corresponds to an arbitrary reference cross section evaluated with a specified reference flux energy spectrum and temperature. FABULOUS computes Bondarenko factors with an analytical expression for flux based on the narrow resonance (NR) and intermediate resonance (IR) approximations:

$$\varphi(E,\sigma_0,T) = \frac{\sigma_0 \varphi_{ref}(E)}{\sigma_t^{(j)}(E,T)+\sigma_0} \tag{8}$$

In this case Eq. (6) reduces to

$$\sigma_{x,g}^{(j)}(\sigma_0,T) = \frac{\int_g \frac{\sigma_x^{(j)}(E,T)\,\varphi_{ref}(E)}{\sigma_t^{(j)}(E,T)+\sigma_0}\,\mathrm{dE}}{\int_g \frac{\varphi_{ref}(E)}{\sigma_t^{(j)}(E,T)+\sigma_0}\,\mathrm{dE}}. \tag{9}$$

The module FABULOUS was modernized to take advantage of the updated integration routines in AMPX and the integrals in Eq. (9) are now solved using the Runge-Kutta method with adaptive step size[7]. There are two methods available in AMPX to calculate the cross section data in the URR. The module PRUDE employs a method developed by R. N. Hwang at Argonne National Laboratory for calculating unresolved cross sections as a function of energy[10]. In the unresolved resonance region

(URR), average resonance parameters are provided for the SLBW formalism, and the resonance widths are distributed according to a chi-squared distribution with a specified number of degrees of freedom. Flux weighted cross section values can be calculated over an evaluator-specified energy interval using the unresolved resonance parameters. In the averaging process, the method by Hwang makes use of the NR approximation, and the resulting expressions for the average cross section values can be expressed in terms of fluctuation integrals that are also defined in terms of the Doppler broadening ψ and χ resonance line shape functions. In this case Eq. (9) is used. However, in the URR, values for $\sigma_x^{(j)}(E,T)$ are substituted by $\sigma_x^{(j,urr)}(E,T,\sigma_o)$ as calculated by PRUDE. The integration routine is unchanged, as the cross section substitution happens prior to integration. The other method used in the URR calculates probability tables, which is done in the AMPX module PURM[11]. These probability tables are used in the CE libraries. If the probability table is used, $\sigma_{x,p}^{(j)}(E,T)$ is the cross section for the band p of the probability table for reaction x and nuclide j. The probability for a given band is given by P_p. In this case, FABULOUS calculates $\sigma_{x,g}^{(j)}(\sigma_0,T)$ as

$$\sigma_{x,g}^{(j)}(\sigma_0,T)=\frac{\int_g \Sigma_p P_p \frac{\sigma_{x,p}^{(j)}(E,T)\varphi_{ref}}{\sigma_{t,p}^{(j)}(E,T)+\sigma_0}dE}{\int_g \Sigma_p P_p \frac{\varphi_{ref}}{\sigma_{t,p}^{(j)}(E,T)+\sigma_0}dE}. \tag{10}$$

If the URR starts or ends within a group, the numerator and denominator each will have two terms, one containing the sum over the probability table bands, and one using the integral with the point-wise cross section data. Using the same probability tables in the CE and MG library makes the results in SCALE more consistent.

The updated FABULOUS can use the data from PURM as well as PRUDE, but for the MG libraries distributed with SCALE 6.2 probability tables are used to calculate the f-factors in the URR.

The module FABULOUS has been updated to calculate the f-factors for the removal cross section, which is a measure of elastic scattering staying in the group. The removal cross section is defined as

$$\frac{1}{\int_g \varphi(E,T,\sigma_0)dE}\int_g dE\sigma_2^{(j)}(E,T)\varphi(E,T,\sigma_0)\int_{E\prime=E_g}^{E} f_0(E,E')dE', \tag{11}$$

where the definitions are as given before, and E_g is the lower group boundary. Outside the thermal range, elastic scattering does not scatter to exit energies larger than the incident energy; therefore, the inner integral can be extended to the upper energy bound. This makes the removal cross section in the infinite diluted limit the same as the diagonal elements of the scattering matrix for the elastic cross section at Legendre order zero.

Using the NR flux defined in Eq. (7) the NR removal cross section can be calculated as a function of temperature and background value:

$$\frac{1}{\int_g \frac{\varphi_{ref(E)}}{\sigma_t^{(j)}(E,T)+\sigma_0}dE}\int_g \frac{\sigma_2^{(j)}(E,T)\varphi_{ref(E)}}{\sigma_t^{(j)}(E,T)+\sigma_0}dE\int_{E\prime=E_g}^{E} f_0(E,E')dE'. \tag{12}$$

As before, two options are available to calculate the cross section data for the elastic cross section in the URR and both options are available in the updated FABULOUS.

2.4 EXPANDED PROCESSING FOR EXIT ENERGY COVARIANCE DATA

The module PUFF-IV is used to generate covariance matrices with respect to the group-averaged cross section data. With the release of ENDF/B-VII.1, covariance information with respect to the exit energy distribution for fission (χ-distribution) has become available. The SCALE covariance library has always contained covariance information for χ-distributions for selected nuclides. Before the release of ENDF/B-VII.1, the fission spectrum covariance data was constructed by assuming that the distribution can be described by a Watt spectrum and propagating uncertainties on the Watt spectrum parameters[12]. With the release of ENDF/B-VII.1, the χ-distribution covariance data are given in File 35 in an ENDF file for a range of incident energies. The data format does not allow for correlations between different incident energies. Covariance matrices may be given for several ranges of incident energies. The covariance matrix is given on an evaluator-defined exit energy bin structure. The covariance matrix is given for bin probability and not on the bin-averaged probability function. This is different from the cross-section covariance data due to the normalization requirement on the exit-energy distribution. Therefore, a different procedure is needed to convert the evaluator-defined exit energy structure to the user-desired MG structure. The group-averaged one-dimensional χ-distribution for group g'_I ($\chi_{g'_I}$) is defined as:

$$\chi_{g'_I} = \int_{E' \in g'_I} f(E, E')\, dE' \tag{13}$$

with the exit energy distribution normalized as

$$\int_0^\infty f(E, E')\, dE' = 1, \tag{14}$$

and the covariance matrix element between groups I and J is given as

$$\langle \delta\chi_{g'_I}, \delta\chi_{g'_J} \rangle. \tag{15}$$

Since χ is normalized to 1, combining two groups into one group simply implies adding the values for the two groups; therefore, the same applies for the covariance:

$$\langle \delta\chi_{g'_I}, \delta\chi_{g'_J} \rangle = \sum_{I' \in I, J' \in J} \langle \delta\chi_{g'_{I'}}, \delta\chi_{g'_{J'}} \rangle. \tag{16}$$

If splitting a larger group into several groups, χ scales with the bin width, i.e.,

$$\begin{aligned} \Delta E_I &= \sum_{i \in I} \Delta E_i \\ \chi_{g'_I} &= \sum_{i \in I} \chi_{g'_i} \frac{\Delta E_i}{\Delta E_I}, \end{aligned} \tag{17}$$

and the covariance elements scale similarly with the bin.

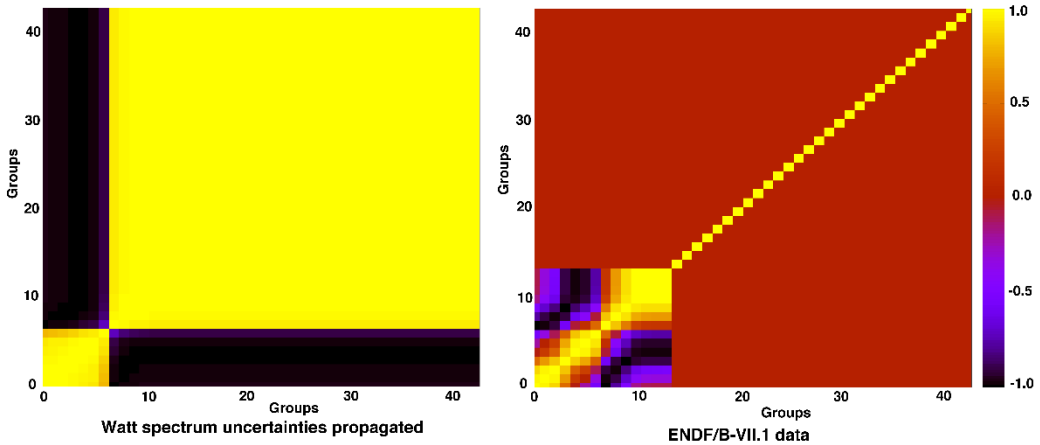

Figure 1. χ-Correlation Matrices for ^{235}U from ENDF/B-VII.1 and Propagated from a Watt Spectrum Parameter. χ Cross Section is Zero for Groups 15–44.

We updated PUFF-IV to process File 35 data and save them into a user-desired, group-averaged covariance format. The covariance data in the ENDF-formatted file are given as a function for incident energy. However, the SCALE covariance file format does not allow for a dependence on incident energy. Therefore, we select the covariance matrix given for the average energy of fission which is calculated as follows: If ν is nu-bar, f is fission, and w is the appropriate flux, the average energy of fission is calculated as

$$10^7 \exp\left(-\frac{\sum \nu f w \frac{1}{2}\left(\log\left(\frac{10^7}{E_{g1}}\right) + \log\left(\frac{10^7}{E_{g2}}\right)\right)}{\sum \nu f w} \right), \tag{18}$$

and the sum is over all groups, and E_{g1} and E_{g2} are the group boundaries for group g.

ENDF/B-VII.1 contains covariance matrices for the χ-distribution for almost all actinides, which are included in the new SCALE covariance library. Figure 1 shows a comparison of the correlation matrix for the χ-distribution in ^{235}U, propagated from the Watt spectrum parameters and as given in ENDF/B-VII.1.

3. NUCLEAR DATA LIBRARY UPDATES AND TESTING WITH SCALE

3.1 MG LIBRARIES

New ENDF/VII.1 MG libraries were generated using the modernized AMPX modules with 252 and 56 neutron groups respectively. The base weighting function for processing MG data of actinide materials (Z > 89) was computed by the point-wise transport code CENTRM for a PWR lattice at 300K. The standard weighting function is used for materials with Z<90. The thermal energy range, which includes up-scattering reactions, was extended to 5 eV, compared to 3 eV in the previous SCALE MG libraries. Temperature-dependent thermal-scattering matrices for water-bound H, ^{16}O, and actinide materials were processed with temperature-dependent thermal flux spectra obtained from CENTRM calculations for a PWR pincell. Actinide and ^{16}O MG thermal scattering kernels were weighted with the fuel zone flux at temperatures of 293K, 600K, 900K, 1200K, and 2400K, and the water scatter kernels were weighted with the moderator flux at 293K, 500K, 600K, 650K, 900K, and 1200K. All other thermal scattering matrices at all temperatures were weighted with a temperature-independent Maxwellian spectrum. Group-dependent intermediate resonance (IR) parameters ("lambdas") were calculated for all nuclides. This allows the Bondarenko self-shielding method in SCALE to use the intermediate resonance (IR) approximation for the 252-group libraries. The number of temperatures for the Bondarenko factors was increased. Shielding factors are tabulated at temperatures 292K, 600K, 900K, 1200K, and 2400K. In addition to the Bondarenko factors normally included for capture, fission, elastic, and total cross sections, self-shielding factors are also included for the MG elastic removal cross section in order to address the impact of resonance reactions on the scattering distribution. In the URR, self-shielding factors were calculated using probability tables. Bondarenko factors for nuclides with atomic masses Z>39 were calculated with CENTRM point-wise flux spectra rather than the analytical NR approximation. Two types of CENTRM models were used. Heterogeneous models of water-moderated lattices spanning the range of expected self-shielding were used to calculate shielding factors for ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{90}Zr, and ^{96}Zr. The CENTRM transport calculations were performed using the method of characteristics for 2D unit cell models. Homogeneous models were used to compute shielding factors for the remaining nuclides with Z>39. These CENTRM calculations were performed for homogeneous media containing the absorber material mixed with hydrogen, and the hydrogen concentration was varied to obtain the desired set of background cross sections.

All KENO input files used in the SCALE 6.1 validation report[13] have been rerun with the new libraries and compared with previous results to ensure that the k-eff values are still within expected limits.

3.2 CE LIBRARIES

In order to keep the on-disk size small, the number of points for the point-wise data is kept to a minimum. For that reason, point-wise cross section data were thinned such that eliminated points can be interpolated with a tolerance of 0.1%. The same thinning is not done for MG, as the number of points does not affect the final size of the MG library. However, in the case of nubar, the thinning was too aggressive and impacted the result. In the case of a bare uranium sphere of radius 5.9838 cm and enrichment of 98% ^{233}U, 1% ^{234}U, 0.03% ^{235}U and 0.6% ^{238}U the k-eff calculated by MCNP is about 400pcm higher than calculated in KENO-Va. Eliminating the thinning for the CE libraries led to a small increase in on-disk size of the libraries, but led to consistent k-eff values for bare uranium sphere between MCNP and CE and MG KENO-Va calculations. All actinides in the CE libraries have been updated to eliminate the thinning of the cross section data.

The CE libraries support probability tables. In the current ENDF format, cross section data for total, elastic, capture, fission and discrete inelastic to the first exited state (MT=51) can be given by resonance parameter in the unresolved range. Therefore, probability tables can be calculated for these reactions. Fission and MT=51 will only be given if they are energetically allowed. Previously, KENO-Va expected to have probability tables for total, elastic, capture and fission. As a result, the probability table for fission was present even if the fission cross section is zero. Probability tables for any other reactions could not be saved in the CE library. The KENO-Va code as well as the AMPX modules were updated to allow a variable number of probability tables in the CE library. This way an empty table for fission does not need to be stored and a table for MT=51 can be added. The latter reaction opens in the URR region for ^{238}U. The CE libraries have been updated to include the MT=51 probability table for ^{238}U.

All KENO input files used in the SCALE 6.1 validation report[13] have been rerun with the new libraries and compared with previous results to ensure that the k-eff values are still within expected limits.

3.3 COVARIANCE LIBRARIES

Covariance libraries for release with SCALE 6.2 were generated. These libraries are primarily based on ENDF/VII.1 data. If covariance data are not available in ENDF/VII.1 the same data as in the previous SCALE covariance library were used. Covariance data for the exit energy range (χ-distribution) were augmented with data from JENDL3.3, as not all actinides in ENDF/VII.1 have exit energy distributions. Covariance libraries were produced with 56 and 252 neutron groups. SCALE also includes a program, SAMPLER, which performs statistical sampling from the cross-section data. In order to use the new covariance library in this program, a library of 1000 random samples for the cross-section data was needed. The library of random samples was prepared for the 56 and 252 group library, where the 56-group library is the default library to be used in SCALE 6.2. The updated covariance libraries have been tested prior to release with SCALE 6.2. Testing has been reported at the ICNC-2015 conference in Charlotte[14].

4. INTERNATIONAL COLLABORATIONS

The NEA as well as IRSN are interested in generating MG and CE libraries for SCALE using the JEFF library[15]. With the release of SCALE 6.2, both of which distributed with AMPX, it has now become possible for groups outside of ORNL to produce libraries for SCALE. Carlos Javier Diez (OECD/NEA Data Bank visited ORNL for two weeks to collaborate on the processing of JEFF3.2 with AMPX.

Raphaelle Ichou (IRSN) visited ORNL for two weeks to investigate the possible use of AMPX in her group at IRSN.

5. SUMMARY

In summary, the NCSP FY2015 AMPX Maintenance and Modernization funds have been used to modernize modules X10, FABULOUS, and SIMONIZE. These modules are used in processing MG libraries and have allowed ORNL to add new capabilities. The new modular design made it easy to add the capability to produce f-factors in the URR from probability tables. This allows the use of the same URR treatment for the CE and MG libraries. Capabilities to add f-factors for removal cross-section data have also been added. These enhanced capabilities have been used to generate new ENDF/VII.1 MG libraries, and these new cross-section data libraries will be released with the SCALE 6.2 in FY2016. In addition, we added the capability to process covariance data from χ-distributions that are now available in ENDF/VII.1 evaluations. The updated covariance libraries to be released with the SCALE 6.2 contain those covariance data processed from ENDF/VII.1.

6. REFERENCES

1. D. Wiarda, M. L. Williams, C. Celik, M. E. Dunn, *AMPX-2000: A Cross-Section Processing System for Generating Nuclear Data for Criticality Safety Applications*, International Conference on Nuclear Criticality Safety (ICNC 2015)

2. *SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design*, ORNL/TM-2005/39, Version 6.1, June 2011. Available from the Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-785.

3. "Evaluated Nuclear Data File (ENDF)," Database Version VII.0, url http://www.nndc.bnl.gov/endf/index.html, National Nuclear Data Center, Brookhaven National Laboratory Associated Universities, Inc., Upton, Long Island, New York.

4. D. Wiarda, C. Celik, M. Williams, and M. E. Dunn, C. R. Daily, "NCSP FY 2013 AMPX Annual Report," ORNL/LTR-2014/32, December 2014.

5. C. M. Mattoon, B. R. Beck, N. R. Patel, N. C. Summers, G. W. Hedstrom, *Generalized Nuclear Data: A New Structure (with Supporting Infrastructure) for Handling Nuclear Data*, Nuclear Data Sheets 113(12), pp. 3145–3171 (2012).

6. N.M. Larson, Updated User's Guide for SAMMY*:* Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations, ORNL/TM-9179/R6 (July 2003).

7. W. H. Press, W. T. Vetterling, S. A. Teukolsky and B. P. Flannery, *Numerical Recipes in FORTRAN The Art of Scientific Computing*, Second Edition, Cambridge University Press, 1992.

8. *ENDF-6 Formats Manual: Data Formats and Procedures for the Evaluated Nuclear Data Files ENDF/B-VI and ENDF/B-VII*, eds. M. Herman and A. Trkov, Report BNL-90365-2009 Rev.1

9. M. L. Williams, *Resonance Self-Shielding Methodologies in SCALE 6*, Nucl. Technol. 174, 149 (2011).

10. R. Hwang, *A Rigorous Pole Representation of Multilevel Cross-sections and Its Practical Applications*, *Nuc. Sci. Eng*., **96**, 192, 1987

11. M. E. Dunn, L. C. Leal, *Calculating Probability Tables for the Unresolved-Resonance Region Using Monte Carlo Methods*, PHYSOR 2002 # A0107, May 2002

12. Bryan L. Broadhead and J. J. Wagschal, "The Fission Spectrum Uncertainty," 95821.pdf in *Proc. of PHYSOR 2004—The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments*, April 25–29, Chicago, Illinois (2004).

13. W. J. Marshall and B. T. Rearden, *Criticality Safety Validation of SCALE 6.1*, ORNL/TM-2011/450, Oak Ridge National Laboratory, Oak Ridge, Tenn., November 2011.

14. W. J. Marshall, M. L. Williams, D. Wiarda, B. T. Rearden, M. E. Dunn, D. E. Mueller, J. B. Clarity *Development and testing of neutron cross-section covariance data for SCALE 6.2*, International Conference on Nuclear Criticality Safety (ICNC 2015)

15. OECD/NEADataBank,*JEFF-3.2EvaluatedDataLibrary-Neutrondata*(2014),http://www.oecd-nea.org/dbforms/data/eva/evatapes/jeff_32/