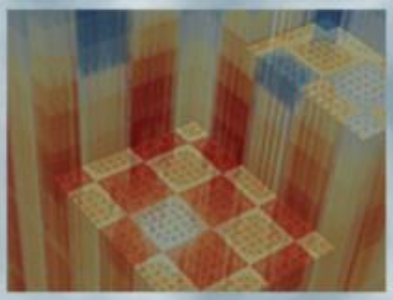
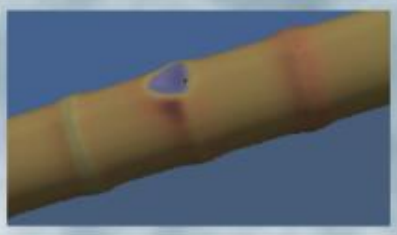
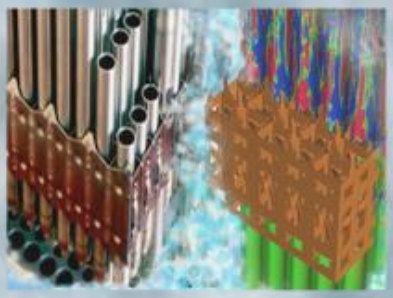
CASL-U-2017-1326-000
ORNL/TM-2017/247

Software Quality Assurance and Verification for the MPACT Library Generation Process

Revision 0

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May 10, 2017

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

REVISION LOG

Revision	Date	Affected Pages	Revision Description
0	5/1/2017	All	Initial version

Export Controlled None

IP/Proprietary/NDA Controlled None

Sensitive Controlled None

Unlimited All Pages

Requested Distribution:

To: N/A

Copy: N/A

Reviewed by:

Date:

Reviewer:

EXECUTIVE SUMMARY

This report fulfills the requirements for the Consortium for the Advanced Simulation of Light-Water Reactors (CASL) milestone L2:RTM.P14.02, "SQA and Verification for MPACT Library Generation," by documenting the current status of the software quality, verification, and acceptance testing of nuclear data libraries for MPACT. It provides a brief overview of the library generation process, from general-purpose evaluated nuclear data files (ENDF/B) to a problem-dependent cross section library for modeling of light-water reactors (LWRs). The software quality assurance (SQA) programs associated with each of the software used to generate the nuclear data libraries are discussed; specific tests within the SCALE/AMPX and VERA/XSTools repositories are described. The methods and associated tests to verify the quality of the library during the generation process are described in detail. The library generation process has been automated to a degree to (1) ensure that it can be run without user intervention and (2) to ensure that the library can be reproduced. Finally, the acceptance testing process that will be performed by representatives from the Radiation Transport Methods (RTM) Focus Area prior to the production library's release is described in detail.

The software quality for the library generation process has improved significantly over the past 18 months. Several independent evaluations of the AMPX, SCALE/AMPX, and VERA portions of the process were a primary mechanism for this improvement. These evaluations (1) enhanced knowledge transfer among technical staff members, (2) increased mutual understanding of the status and capability of each software component, and (3) guided the development of improvements. During this process, all software was included in an ORNL SQA program. Unit and/or regression tests were established for each package, and many software bugs were fixed. The library generation process was automated to ensure integrated testing of all components, as well as reproducibility of the final product. Automation also provided an ingrained level of inherent documentation.

As the quality of the library generation process improved, the rigor of acceptance testing increased. A suite of eight sets of comparisons of MPACT results with continuous energy (CE) Monte Carlo solutions provides a clear basis for identifying errant data or data trends that reveal discrepancies in the final library. CASL stakeholders can review these comparisons and see benefits of a given library compared to previous versions. This establishes a clear pathway from library development to application within VERA and eventual release with MPACT.

However, many important objectives remain to improve the quality of the library generation process, as discussed herein.

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FIGURES

TABLES

ACRONYMS

1D	one-dimensional
2D	two-dimensional
AMA	Applications, Modeling, and Analysis Focus Area of CASL
AMPX	resonance processing code; no longer an acronym
BONAMI	IR cross section code in SCALE
BWR	boiling water reactor
CASL	Consortium for Advanced Simulation of Light Water Reactors
CE	continuous energy (as in cross sections)
CENTRM	pointwise transport code in SCALE
DBRC	Doppler-broadening rejection correction
ENDF	evaluated nuclear data file
ESSM	embedded self-shielding method
FP	fission product
GUI	graphical user interface
IR	intermediate resonance
IRFFactor	cross section processing code in SCALE
JEFF	OECD-NEA coordinated Joint Evaluated Fission and Fusion nuclear data
JENDL	Japanese evaluated nuclear data library
KERMA	kinetic energy released in matter
KENO	Monte Carlo code in SCALE
LWR	light-water reactor
MCNP	Monte Carlo N-Particle
MERIT	pointwise slowing down and ESSM code in VERA/XSTools
MG	multigroup (as in cross sections)
MOC	method of characteristics
MPACT	radiation transport code in VERA; no longer an acronym
MWD	megawatt-day
NJOY	nuclear data code
NR	narrow resonance
ORIGEN	Oak Ridge Isotopic Generation code in SCALE
ORNL	Oak Ridge National Laboratory
PW	pointwise
PWR	pressurized water reactor
RI	resonance integral
RTM	Radiation Transport Methods Focus Area in CASL
SAMPX	Simplified AMPX
SCALE	Standardized Computer Analyses for Licensing Evaluations code
SG	subgroup
Shift	Monte Carlo code in SCALE
SNU	Seoul National University
SPH	super-homogenization
SQA	software quality assurance
TPL	third-party library
V&V	verification and validation
VERA	Virtual Environment for Reactor Applications
VERA-CS	VERA Core Simulator
XS	cross section

1. INTRODUCTION

The MPACT [MPA15] neutronics code within the Virtual Environment for Reactor Analysis (VERA) [Tur16] code suite is being developed by the Consortium for Advanced Simulation of Light Water Reactors (CASL) [CAS15]. MPACT provides a three-dimensional (3D) full-core neutron transport solution with isotopic depletion/decay by coupling with the SCALE/ORIGEN [Rea16, Sect. 5.1] code. MPACT primarily uses the subgroup method for resonance self-shielding [Gol62, Sta98], using a cross section library based on ENDF/B-VII data [Cha11]. These data have been processed using the AMPX [Wia16] and SCALE [Rea16] code packages, along with a few other CASL utility programs.

This report summarizes and borrows liberally from several key CASL reports describing the library generation process [Kim15a] and benchmarking of the latest releases of the library [Kim17b] and documents to describe:

- an overview of the library generation process (Sect. 2);
- software quality assurance (SQA) practices associated with this cross section library generation process (Sect. 3);
- verification testing of the library during the generation process (Sect. 4);
- automation of that process to improve repeatability (Sect. 5);
- benchmarking of the final product through comparison with continuous-energy (CE) Monte Carlo codes (Sect. 6); and
- conclusions on the current status of the library generation process and consideration for future work (Sect. 7).

The data used by ORIGEN include isotopic decay data and problem-independent cross sections based on data from ENDF/B, JEFF [San09], and JENDL [Shi11], as well as problem-specific reaction rate information passed from MPACT for a select set of ENDF nuclide reactions from the MPACT library. While this report covers the MPACT library, it does not cover the additional ORIGEN data which are documented in detail in Sect. 5.1 of the *SCALE Code System* [Rea16].

This report fulfills the requirements for CASL milestone L2:RTM.P14.02, “SQA and Verification for MPACT Library Generation,” that has the following completion criteria: “A report will be delivered that documents the verification testing and software quality status, along with the future work required for generation of an MPACT library with full automation and verification” per the following description:

> *This milestone is to continue to improve the automation and software quality of the MPACT library generation process and document the status in a MPACT Cross Section Library Verification report that contains clear metrics on the software quality, automation, repeatability, verification, and benchmarking. The software quality will define the location of repositories, a listing of unit and regression tests with a clear description of their coverage.*

The automation will describe the process and extent to which the cross section libraries may be automatically generated with a single script. Absent of complete automation, repeatability will document the manual executions required to generate a library and provide feedback from someone creating a library for the first time from processed CE data. Verification will document the tests used in the library generation process that ensure internal consistency and consistency of the final product with the codes that generated it. Finally, benchmarking will compare the MPACT results with CE Monte Carlo and include an assessment based on target accuracies.

2. OVERVIEW OF THE LIBRARY GENERATION PROCESS

The cross section library generation process is documented in detail in *AMPX-6: A Modular Code System for Processing ENDF/B* [Wia16], and *Procedure to Generate the MPACT Multigroup Library* [Kim15a]. The process includes four main sections that use software from two code suites—SCALE with AMPX and VERA with XSTools and MPACT—as detailed below:

- AMPX processing of ENDF/B-VII data to create a CE AMPX library;
- AMPX processing of the CE AMPX data to generate a problem-independent multigroup (MG) AMPX library;
- AMPX processing of problem-independent MG AMPX data to improve the MG AMPX library and to include subgroup data for a class of problems; and
- Incorporation of supplemental data with the MG AMPX library and organization into a format readable by MPACT.

2.1 CONTINUOUS ENERGY (CE) AMPX LIBRARY

The well-documented AMPX process to generate a CE library from the ENDF/B-VII.0 and ENDF/B-VII.1 data [Wia16] is designed to provide CE data in a usable format that replicates the original data. This results in a cross section library usable by CE Monte Carlo such as Shift [Pan15] and KENO [Rea16, Sect. 8.0], and deterministic transport codes such as CENTRM [Rea16, Sect. 7.4]). These data are produced at a series of specific material temperatures that are stored on the library.

By leveraging consistent CE data, verification testing can be performed using Shift or KENO to evaluate the accuracy of the MG MPACT library with the SG resonance processing in MPACT at specific temperatures. Shift also includes the ability to account for variations between the temperatures available on the library.

2.2 PROBLEM-INDEPENDENT MULTIGROUP (MG) AMPX LIBRARY

The conventional AMPX process to generate a problem-independent MG library from CE data leverages a series of approximate neutron spectra to serve as weighting functions to compute temperature-dependent microscopic cross sections for a specific energy group structure. The approximate spectra are progressively improved from very basic shapes in energy (e.g. Maxwellian) to complex (e.g. self-shielded, temperature-dependent), ultimately providing a problem-independent library designed to be used with a problem-specific resonance processing step. Key portions of the problem-independent library will be replaced using an improved spectrum before generation of the final deterministic transport solution. Figure 2.1 depicts the procedure to generate a problem-independent MG AMPX library.

The initial approximate spectrum is composed of a fission spectrum in the high-energy range, a 1/E spectrum in the resonance range, and a Maxwellian spectrum in the thermal

scattering range. This approximate spectrum provides an initial estimate for the one-dimensional (1D) and two-dimensional (2D) scattering cross sections. This initial spectrum is supplemented by generating homogeneous F-Factors for each isotope to provide cross section data as a function of the background cross section using homogeneous Bondarenko F-factors for homogeneous mixtures with ^{1}H and target nuclide. These updated F-Factors provide improved data for use with an intermediate resonance (IR) Bondarenko method, as found in BONAMI [Rea16, Sect. 7.3]. In addition, XSDRN was used to solve a simple fission-spectrum-in-water problem to define the transport cross section in hydrogen using the method described in *Investigation of Neutron Leakage Conservation Method to Generate H-1 Transport Correction Factors* [Kim17a].

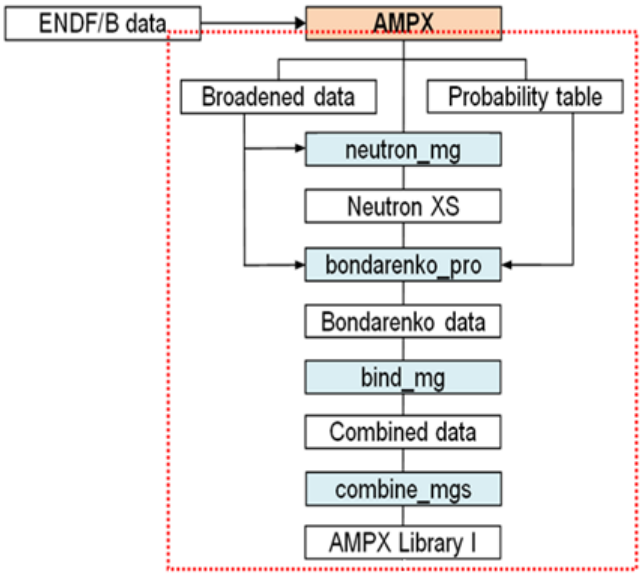


Figure 2.1. Flow Chart of the AMPX Procedure for Generating the VERA MG Library.

Generation of the CE and MG libraries for SCALE/AMPX primarily uses the EXSITE [Wia16] graphical user interface (GUI) to read a set of template files and generate SCALE/AMPX inputs for individual isotopes. Then SCALE/AMPX is run for each of the inputs, and at several intermediate steps throughout the process, individual outputs are collected together to form an AMPX library.

2.3 IMPROVED MG AMPX LIBRARY WITH SUBGROUP DATA

SCALE is a general geometry neutronics code used for a wide variety of problems. Therefore, XSProc [Rea16, Sect. 7.1] uses the MG AMPX library to generate problem-specific cross section data using BONAMI in conjunction with a pointwise (PW) slowing down calculation from CENTRM [Rea16, Section 7.4] for each unique pin cell specification (geometry, material, temperature, Dancoff factor). However, this can lead to long execution times and substantial user-burden in decomposing the problem into pin cell types. In contrast, MPACT is designed to use a cross section library generated for a

particular class of problems. This allows for additional processing at the library-generation stage that can reduce the execution time experienced by the MPACT user. For CASL, the class of problems is limited to thermal-spectrum LWRs with oxide fuel.

As with homogeneous F-Factors in a problem-independent MG library, AMPX will also generate heterogeneous F-Factor data for a suite of pin cells. Figure 2.2 depicts the SCALE/AMPX library generation procedure that includes the heterogeneous F-Factor generation to improve resonance data through homogeneous and heterogeneous F-Factors. For each nuclide, each pin cell represents an additional data point on a plot of the F-Factor at a particular background cross section. For CASL, this includes pin cell problems that range in geometry, enrichment, and density, but all contain borated water, Zircaloy cladding, helium-filled gap, and UO_2-based fuel in a square lattice. A monotonic-spline or least-squares fitting routine computes a smooth F-Factor model as a function of background cross section.

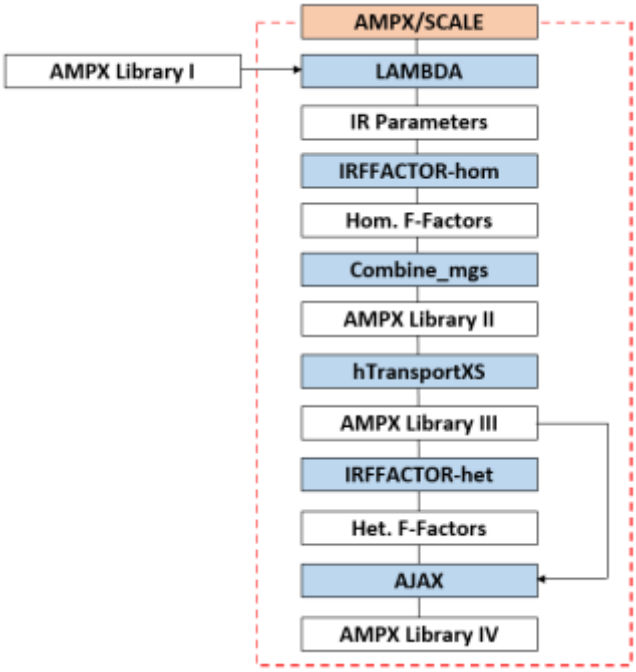


Figure 2.2. SCALE/AMPX Process for Generating a Problem-Dependent Library.

In addition, the SUBGR code [Kim16a] is included in AMPX so that the levels and subgroup weights (as a function of temperature) can be generated. SUBGR post-processes the heterogeneous F-Factors into a set of subgroup levels and weights for use in an MPACT subgroup calculation. Figure 2.3 depicts the procedure to generate subgroup data, which are added to a full AMPX library. If a different class of problems were to be considered, the user would need to establish a new suite of heterogeneous pin cells to bound the typical range of materials and geometries.

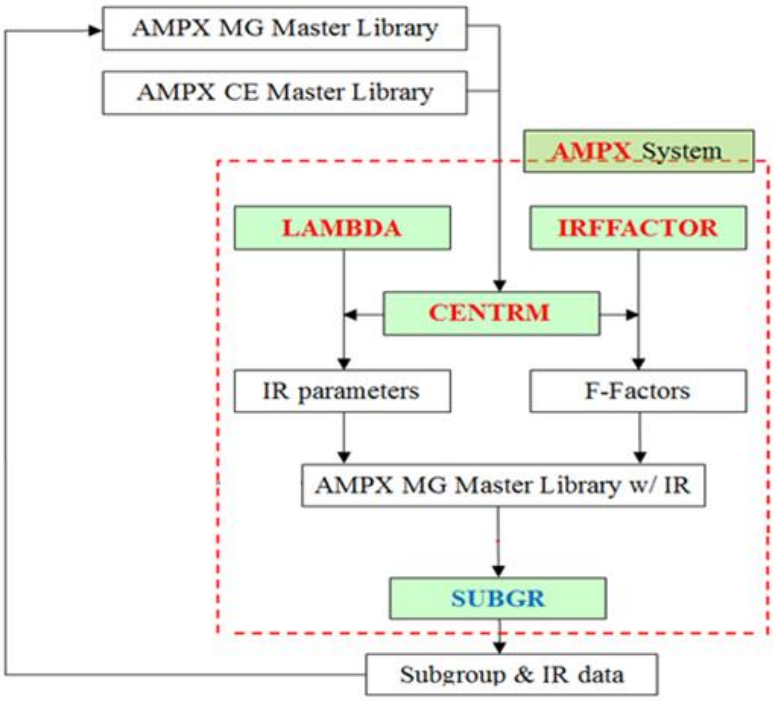


Figure 2.3. MPACT Library Generation Procedure.

2.4 SUPPLEMENTAL DATA AND LIBRARY FORMATS

MPACT can read either a simplified AMPX (SAMPX) [Kim17b] format or the native MPACT format. While the MPACT library format is similar to the DeCART [Cho02] format, the SAMPX format extends the MG AMPX library. In addition to the data provided on the AMPX library, additional data must be added to the SAMPX or MPACT library because all of the required information is not yet available in the AMPX-processed MG library. At this writing, data needed include the time-dependent data, some heat-generation (κ) values, supplemental data to account for resonance upscattering, and the super-homogenization (SPH) adjustments. This lack of data is an obstacle to developing an automatic procedure to generate the MG MPACT and SAMPX library. Since the MPACT format library includes resonance data only for specific nuclides and energy groups, representative energy- and nuclide-dependent background cross sections must be provided to obtain shielded resonance cross sections for nonresonance groups and nuclides. Therefore, the SAMPX format library was developed to directly use the MG AMPX library as an interim step.

The six-group time-dependent data associated with the delayed neutron fractions (β_g) and their decay constants (Λ_g) will be added to the MG AMPX library in the future. These data are generated by the SCALE data team using the NJOY code system [Mac94].

The MPACT format library contains a single set of κ values to compute the energy-generation: an effective recoverable energy from fission and capture that incorporates an estimate of the energy release from the captured neutrons. The SAMPX library includes two additional sets: the recoverable energy release from neutron fission and the recoverable energy release from neutron capture.

CE-KENO includes an option to account for resonance upscattering and was used to generate corrections to the MPACT data. To complete the resonance cross section table, MERIT was used to compute background cross sections. MERIT is maintained in revision control within VERA/XSTools and is comparable to the AMPX IRFFactor package. Then the resonance cross section tables were converted into the subgroup data through least square fitting by SUBGR. This was completed using an independent execution, and the data were added to the SAMPX/MPACT library as an optional parameter. The resonance upscattering data are available for use in MPACT and were used to model the Watts Bar Unit 2 xenon transient. However, members of CASL's Applications, Modeling, and Analysis (AMA) Focus Area have decided not to use these data for production analyses because the comparison to operational data is less accurate with it enabled. This will require further investigation.

The generation of the SPH factors is a more manual process and requires the use of codes outside of SCALE. CE-KENO is used to generate a set of reaction rates for each isotope, temperature, and group for a suite of various pin cell problems used in the IRFFACTOR heterogeneous models. The SPH factors are chosen to conserve reaction rates obtained by the MPACT P_2 results with the original MG MPACT library to be consistent with the KENO reaction rates. Future work will include an evaluation of the use of TCP0, rather than P_2 scattering. Figure 2.4 provides the SPH factors of group-23 (6.25~7.15 eV) for ^{238}U as a function of temperature and background cross sections. This procedure is identical to that used to generate resonance upscattering data. The SPH factors can be selectively applied to energy groups showing large reaction rate differences. For example, the SPH factors were applied to groups 10, 11, 12, 13, 16, 18, 19, and 23 in the SAMPX 51-g library.

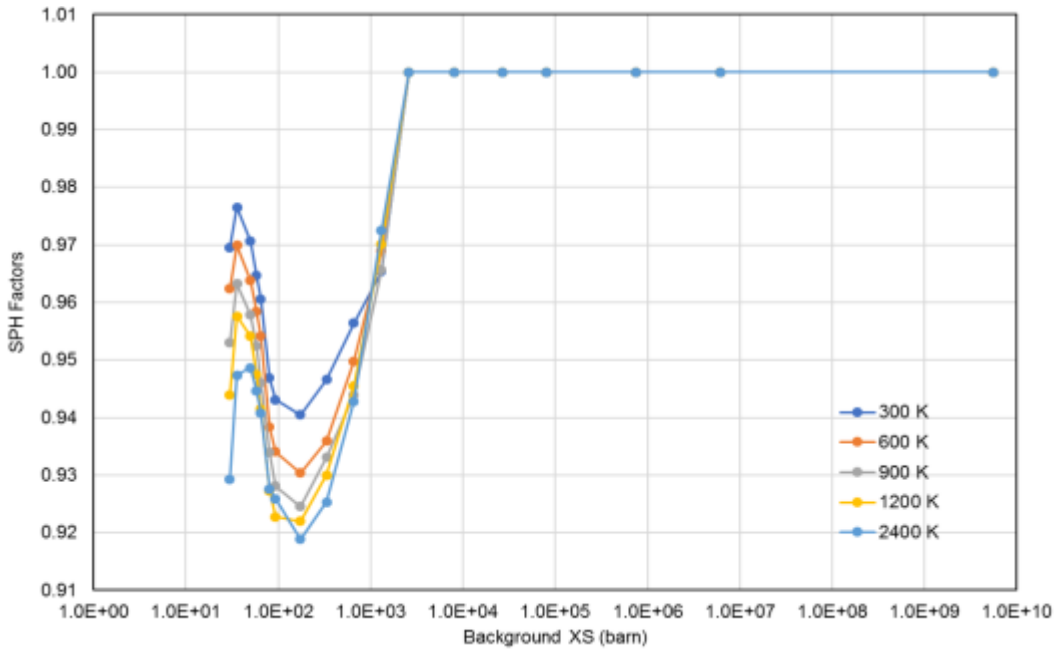


Figure 2.4. SPH Factors for Group-23 Used in SAMPX v5.0.

2.5 FUTURE WORK ON PROCESS INTEGRATION

The following action items are important to completion of the integration portion of the data processing within automatable scripts:

- The MG AMPX library includes the fission and capture κ values. However, the fission κ values are read from the ENDF/B evaluated nuclear data, but they are provided by hard-wired internal values. Therefore, the AMPX code package must be modified to read the fission κ values from ENDF/B.
- The capture κ values in the MG AMPX library are provided by hard-wired internal values. These values were estimated through the KERMA factors by using the NJOY HEATR module with old ENDF/B data. The AMPX code package must include a capability to estimate the KERMA factors to obtain capture κ values.
- The AMPX code package must be improved to generate the time-dependent data to be incorporated into the MG AMPX library.
- The heterogeneous IRFFACTOR procedure must be improved to use either CE-KENO or CENTRM to calculate F-Factors as a function of background cross sections. This procedure can be used in obtaining a resonance cross section table considering epithermal upscattering. Currently, the resonance cross section table with epithermal upscattering is generated by using CE-KENO and MERIT using ESSM. This allows for the removal of the nearly redundant MERIT software from the library generation code suite.
- SUBGR was integrated with AMPX, and the capability was extended to treat the SUBGR data file from the heterogeneous IRFFACTOR. More unit and verification tests should be included.
- The heterogeneous IRFFACTOR must be improved to read external resonance cross section tables to obtain corresponding background cross sections by performing the ESSM calculations. This function can be used in obtaining new resonance cross section tables considering the SPH factors. Currently the MERIT code is used for this.
- A VERA capability must be established to allow for the creation of the data library that includes the generation of SPH and resonance upscatter corrections using MPACT and SCALE/AMPX together.
- The SPH factor generation process should allow for comparison of SPH factors using either TCP0 or P_n scattering.

3. SOFTWARE QUALITY ASSURANCE (SQA)

The AMPX and SCALE codes are maintained within the SCALE Quality Assurance Program [Rea13], while MPACT and XSTools are part of VERA and conform to the CASL QA procedures.

3.1 SCALE/AMPX

The SCALE QA Plan [Rea13] provides specific guidance to all SCALE project staff as to which QA requirements must be met for SCALE operations, identifies who is responsible for meeting those requirements, and details how those requirements are to be accomplished. Among other goals, the processes described in that plan are intended to ensure that:

- routine maintenance and further enhancement of the SCALE code system is performed in a controlled, documented, and traceable fashion;
- qualified personnel perform the SCALE system maintenance and enhancement;
- changes and enhancements are tested, documented, and implemented in accordance with established procedures;
- necessary verification and validation activities are performed; and
- public releases of the code to users are conducted in accordance with established procedures.

The scope of the SCALE QA Plan is limited to those activities required to maintain the operational integrity of the SCALE configuration controlled version, verification, and validation activities which serve to qualify the SCALE system. The SCALE project uses an electronic system (fogbugz) to provide a collaborative development infrastructure, including features for the development backlog, QA workflow, source code version control, document control, bug tracking, helpline, and project management metrics. The scope of these QA activities is detailed in a series of cases in the fogbugz system.

The list of cases that are specific to CASL requirements are tracked in the parent case (#9830[a]), which contains 69 direct child cases, 48 of which are closed, and many grandchild and lower cases. Each case clearly defines an issue (to-do, bug, etc.), evaluation of the priority and requirements, design discussion, software changes, and review. The fogbugz system allows for every software change (commit) to be directly associated with a case to simplify the review process and retain the software changes, along with the ticket describing the requirements and review. Each change associated with the parent case includes a specific unit test verifying the functionality.

The list of cases specific to the general AMPX library generation process is defined in fogbugz with a filter[b] on the AMPX Nuclear Data Development. This currently has 66 open cases and 100 closed cases, with some overlap with the CASL cases.

[a] https://fogbugz.ornl.gov/default.asp?pre=preMultiSearch&pg=pgList&pgBack=pgSearch&search=2&searchFor=9830
[b] https://fogbugz.ornl.gov/default.asp?pg=pgList&pre=preSaveCurrentFilter&ixArea=23

The unit test suite for AMPX includes 177 tests, 7 of which are from SUBGR and 16 from IRFFactor, shown in Table 3.1. As noted later in the automation section, at several stages in the library generation process, the data are evaluated for internal consistency using the RADE module [Wia16]. RADE checks the MG AMPX libraries, including neutron, gamma and coupled neutron-gamma data, for internal consistency.

Table 3.1. SCALE/AMPX Unit and Regression Tests for MPACT Library Generation

Package	Name	Purpose
SUBGR	testSegev	Segev interpolation
	testConmin	Least square fitting based on Conmin
	testFitting0	Least square fitting for RI conservation
	testFitting2	Least square fitting for XS conservation
	testInverse	Inverse matrix
	testSpline	Cubic spline
	TestSubgroupCalc	Subgroup data generation
IRFFactor	fff_montonicUnitTest	Monotonously changing data
	AddBF_data	Computing f-factors for within-group scatter
	tstTransport_Options_fort	Tests for class Transport_Options
	TestHTransportXSParameters	Test for transport XS
	IRFFactorUnitTests	Tests for Routines in IRFFACTOR
	tstRunTransport_fort	Tests for class RunTransport
	TestRunXSProc	Test for XSProc
	tstCell_Builder	Tests for class Cell_Builder
	Shift_API	Tests for class Shift_API
	tstRunShift	Tests for class RunShift
	LambdaTest	Tests for the LAMBDA calculations
	tstTransport_Options	Tests for class Transport_Options
	TestHTransportXSSequence	Tests for hTransportXS sequence
	tstRunTransport	Tests for class RunTransport
	TestHTransportXSModule	Tests for HTransportXS module
	HomoIrfTest	Tests for homogeneous IRFFactor

3.2 VERA/XSTOOLS

The XSTools repository is maintained in version control (git) on casl-dev.ornl.gov and conforms to the standards defined in the CASL SQA Plan [Sie15]. The software contains five packages: AmpxSlib, DecLib, FF2RI, MERIT, and Moc1D. The Moc1D package is no longer used; it has been replaced with the SCALE/AMPX HTransportXS module that uses XSDRN. Moc1D will be removed from the repository. As noted in Section 2.4, MERIT is being used to compute background cross sections to complete resonance cross section tables by performing the ESSM calculations; MERIT will be replaced with the heterogeneous IRFFACTOR. The FF2RI package is a simple program to convert the F-Factors in the AMPX MG library into RIs and print them out for SUBGR. Since SUBGR was already integrated with AMPX, this program will be no longer used. The DecLib package is used to generate the MPACT format library using the MG AMPX library and supplemental data. The MPACT format library includes several drawbacks and limitations and the associated code packages are outside of the AMPX and SCALE code packages. Therefore, the MG AMPX library needs to be used by adding supplemental data which

can be inside the SCALE SQA. The SAMPX library format was developed as an interim format until the MG AMPX library includes supplemental data.

AmpxSlib contains a single regression test that includes an input file, 47-group AMPX and SG data, the time-dependent data, and a separate file for the heat generation (κ) values. It then compiles the MG SAMPX library and compares it with an existing "gold" library. While this is sufficient for testing of the existing capability, the testing of this package should be updated to use the 51-group library. Similarly, the DecLib package contains a single regression test that requires 10 input files and ensures that changes do not alter the solution of this single package for a single test problem (with 47-groups). As the MPACT-formatted library is deprecated, additional verification testing of the DecLib package will not be included. The FF2RI and MERIT codes also include a single regression test that executes the code for a single (47-group) problem and compares the solution with a gold file. These tests are noted in Table 3.2.

Table 3.2. VERA/XSTools Unit and Regression Tests for MPACT Library Generation

Package	Name	Purpose
AmpxSlib	test_01	Generate a sample of the SAMPX 47-g library
DecLib	test_01	Generate a sample of the MPACT 47-g library
FF2RI	test_01	Convert the AMPX MG library and SUBGRdata into a file for SUBGR
MERIT	test_01	Complete resonance XS table by generating background cross sections

3.3 MPACT

MPACT is also maintained within the CASL SQA Plan and the verification and validation has been documented in [CASL-U-2016-1199-000]. As discussed in Section 2.4, for the library generation process, MPACT is used to compute the SPH factors for a particular set of nuclide-group-reactions. This requires MPACT to be solved in the standard, well-verified manner for which it was designed and the results (energy-dependent reaction rates) are also well tested.

3.4 FUTURE WORK FOR SQA OF THE LIBRARY GENERATION CODE

While MPACT and SCALE/AMPX require little additional work to have a mature SQA process, there is substantial work required for the capability in the XSTools repository. Therefore, it is recommended that the following actions take place:

- Deprecation of the Moc1D and FF2RI packages, as they will no longer be used;
- Enhancement of IRFFactor with KENO and/or Shift to compute background cross sections for resonance upscattering and the SPH factors so that MERIT can be deprecated;
- Substantial increase in the unit testing of routines in DecLib; and
- Incorporation of supplemental data into the MG AMPX library and direct use of the MG AMPX library through the AMPX resource in MPACT, so that it does not need to maintain AmpxSlib.

4. VERIFICATION TESTING DURING LIBRARY GENERATION

4.1 VERIFICATION OF THE CENTRM SLOWING DOWN CAPABILITY

Currently, heterogeneous models are being used to generate resonance self-shielded cross section tables as a function of background cross sections by performing the CENTRM slowing down calculation with the MOC (Method of Characteristics) spatial discretization. Verification has been performed for the CENTRM slowing down calculations with MOC and Sn (Discrete Ordinate Method).

Figure 4.1 provides comparisons of reaction rates and microscopic cross section for ^{235}U and ^{238}U between the CENTRM and CE-KENO results for the typical PWR fuel pin. The KENO reaction rates and microscopic cross section were tallied with the SCALE 6.2 252-group structure. There is very good agreement in reaction rates and absorption and nu*fission self-shielded cross sections. This indicates that the CENTRM slowing down capability is working reasonably.

This example problem needs to be added to the SCALE regression testing suite to ensure that future changes to CENTRM and/or CE-KENO do not break this verification test.

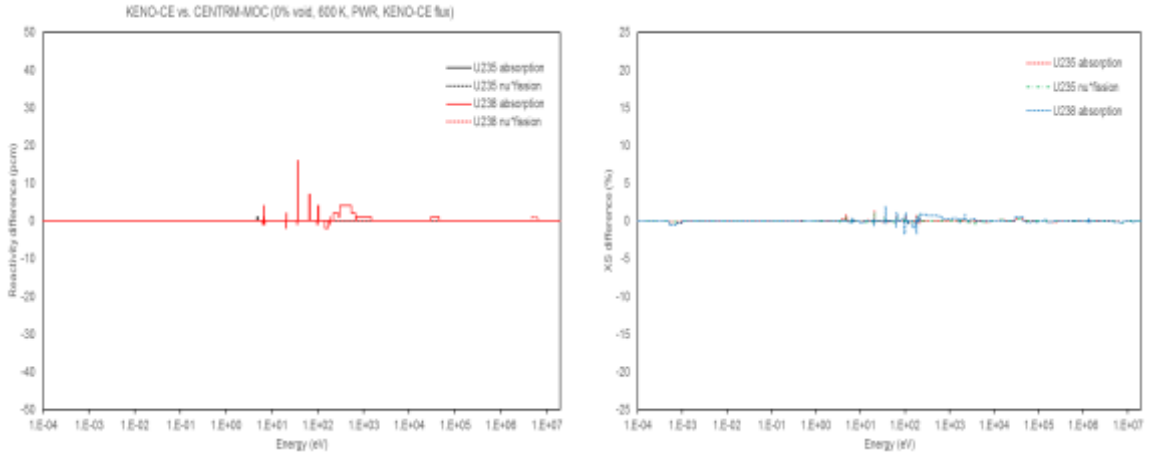


Figure 4.1. Comparisons of Reaction Rate and Cross Sections Differences.

4.2 VERIFICATION OF THE ESSM CAPABILITY IN IRFFACTOR

Resonance cross section tables are completed by computing background cross sections with self-shielded MG cross sections obtained from the CENTRM calculation by performing the ESSM fixed source calculations. The heterogeneous IRFFactor controls the procedure including the slowing down and ESSM calculations. Verification was performed to check if the background cross sections are correctly obtained by performing the ESSM fixed-source calculations. Figure 4.2 provides comparisons of self-shielded absorption cross section tables for important resonance group-23

(6.25~7.15 eV) of ^{235}U in the 51-group structure between IRFFactor and MERIT. This figure shows the data are very consistent with each other.

This example problem must be added to the SCALE regression testing suite to ensure that future changes to CENTRM and/or CE-KENO do not break this verification test.

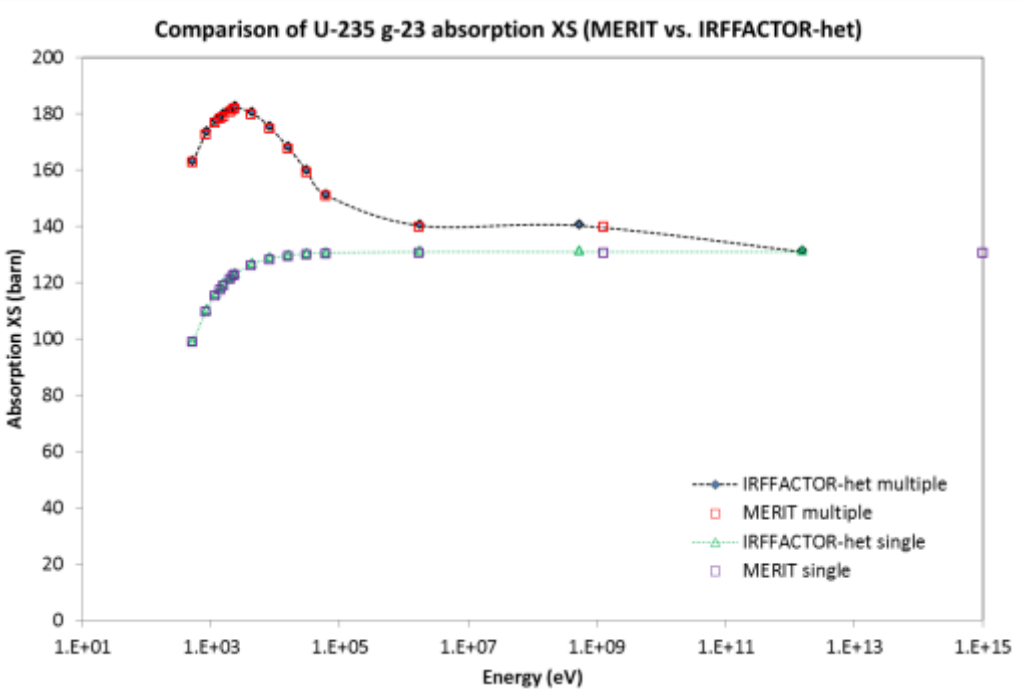


Figure 4.2. Comparison of Self-Shielded XS tables for ^{235}U Group-23 Absorption.

4.3 VERIFICATION OF THE SUBGROUP DATA GENERATION AND USE

The resonance self-shielded cross section tables are converted into subgroup data using the SUBGR program [Kim16a] based on least square fitting which are to be used in estimating problem dependent self-shielded cross sections in MPACT. The SUBGR program includes an internal verification procedure by comparing the reconstructed resonance integrals (RIs) or cross sections (XSs) from subgroup data to the original RIs or XSs. However, the MPACT subgroup module must be verified to correctly estimate self-shield cross sections that are consistent with the original resonance self-shielded cross-section data. The MPACT subgroup module includes a Bondarenko iteration to consider resonance interferences between resonance nuclides. Since resonance self-shielded cross section tables are typically generated without considering resonance interference, the Bondarenko iteration must be skipped for this assessment. Because MPACT does not include a user option to skip the Bondarenko iteration, MPACT was modified to do so for this verification process only. Self-shielded absorption and ν*fission cross sections for ^{235}U and ^{238}U have been estimated by the MPACT subgroup calculations without considering resonance interferences. Figure 4.3 provides comparisons of self-shielded cross sections between MPACT and IRFFactor which are very consistent with each other.

Modifications through MPACT user interface to support this analysis are required so that this example problem can be added to the VERA/MPACT regression testing suite. This will ensure that future changes to do not break this verification test.

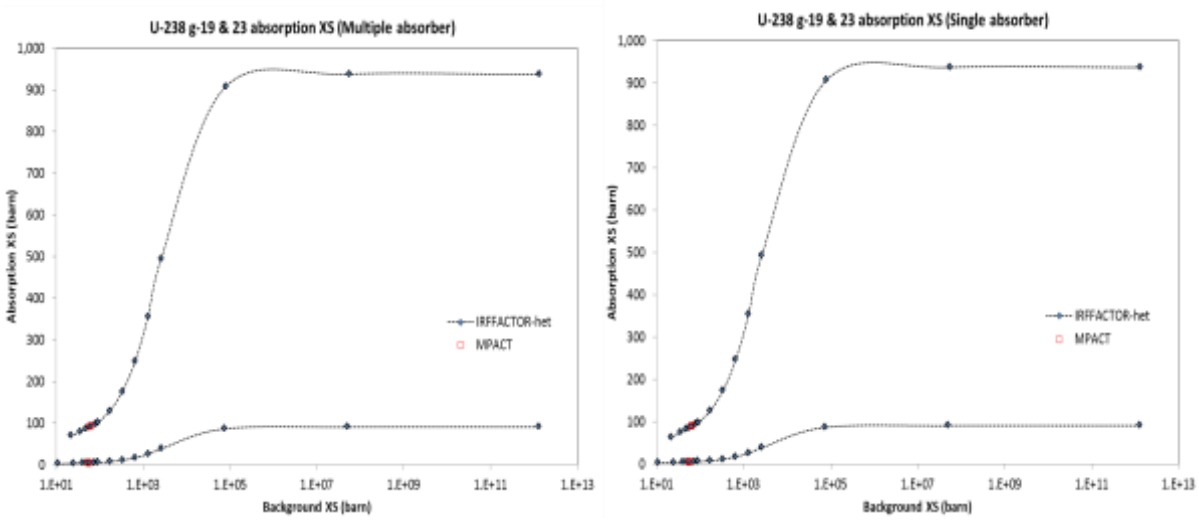


Figure 4.3. Reconstruction of the Self-Shielded Cross Sections by MPACT (^{238}U Groups-19 and -23, Absorption, Single/Multiple Absorber Models).

Investigation has demonstrated that the current CENTRM-MOC is working correctly. However, non-negligible errors persist in predicting the self-shielded cross sections for some of the larger ^{238}U resonances that can contribute 10–20 pcm reactivity error for each resonance in the 252-group structure. On average, the total reactivity by CENTRM-MOC is underestimated by about 100 pcm, which must be improved. The 51-group structure is not optimized, resulting in temperature reactivity bias and larger reactivity differences compared to the 252-group results. Therefore, the 51-g structure must be improved to resolve the temperature reactivity bias and relatively large reactivity errors. Self-shielded cross section tables generated by IRFFACTOR with heterogeneous models are very consistent with those by the MERIT slowing down program, which employs the same ESSM calculation to obtain background cross sections. The AMPX self-shielded cross section tables are being correctly generated by the SCALE/AMPX IRFFACTOR, and the self-shielded cross sections estimated by the MPACT subgroup module are very consistent with the original self-shielded cross section tables prepared by IRFFactor, which indicates that the MPACT subgroup module is working correctly.

Regression tests that verify these results must be added to the SCALE regression testing suite to ensure that future changes to CENTRM and/or CE-KENO do not disrupt this capability.

4.4 AUTOMATIC REACTION RATE ANALYSIS

A valuable tool was added into MPACT for cross section library verification to produce the error of group-wise reaction rate in terms of eigenvalue. This allows the largest sources of error in the cross section library to be quickly pinpointed regarding an isotope, a reaction channel, and an energy group/range. Two candidate methods—the perturbation method and the neutron balance method—are described in ”Automatic Eigenvalue Analysis for Multigroup Cross Section Library Verification” [Liu17]. Since it is obtaining the precise scattering matrix (including high order moments) from the Monte Carlo method is not straightforward, the neutron balance method is implemented for the routine verification of MPACT cross section libraries.

The neutron balance method for eigenvalue analysis was introduced to verify a cross section library and associated resonance methods [Kim15b]. Considering a case with reflective boundary conditions, the eigenvalue can be written as the ratio of neutron production to the neutron absorption,

$$k_{\inf} = \frac{\sum_j \sum_i \sum_g \nu\Sigma_{f,g,i}\phi_{g,j}V_j}{\sum_j \sum_i \sum_g \Sigma_{a,g,i}\phi_{g,j}V_j} \tag{4.1}$$

In Eq. (4.1), i, j, g are the indices of isotope, material region, and energy group, respectively. Estimation of the $k_{\inf}$ error due to an isotopic reaction rate error of group g is given as

$$\begin{cases} \Delta k_{a,g,i,j} = \left(\dfrac{\sum_{j'} \sum_{i'} \sum_{g'} \nu\Sigma_{f,g',i'}\phi_{g',j'}V_{j'}}{\sum_{j'} \sum_{i'} \sum_{g'} \Sigma_{a,g',i'}\phi_{g',j'}V_{j'} + \Delta R_{a,g,i,j}} - k_{\inf}^{ref} \right) \\ \Delta k_{\nu f,g,i,j} = \left(\dfrac{\sum_{j'} \sum_{i'} \sum_{g'} \nu\Sigma_{f,g',i'}\phi_{g',j'}V_{j'} + \Delta R_{\nu f,g,i,j}}{\sum_{j'} \sum_{i'} \sum_{g'} \Sigma_{a,g',i'}\phi_{g',j'}V_{j'}} - k_{\inf}^{ref} \right) \end{cases}. \tag{4.2}$$

All quantities in Eqs. (4.1) and (4.2) except the ΔR term are from the reference Monte Carlo calculation. ΔR can be defined as the reaction rate error between the test and reference results,

$$\begin{cases} \Delta R_{a,g,i,j} = V_j(\Sigma_{a,g,i,j}^{test}\phi_{g,j}^{test} - \Sigma_{a,g,i,j}^{ref}\phi_{g,j}^{ref}) \\ \Delta R_{\nu f,g,i,j} = V_j(\nu\Sigma_{f,g,i,j}^{test}\phi_{g,j}^{test} - \nu\Sigma_{f,g,i,j}^{ref}\phi_{g,j}^{ref}) \end{cases} \tag{4.3}$$

In *Improvement of the VERA Neutronics Simulator MPACT* [Kim15b] another definition of ΔR is presented to isolate the cross section error,

$$\begin{cases} \Delta R_{a,g,i,j} = V_j \phi^{ref}_{g,j} (\Sigma^{test}_{a,g,i,j} - \Sigma^{ref}_{a,g,i,j}) \\ \Delta R_{\nu f,g,i,j} = V_j \phi^{ref}_{g,j} (\nu\Sigma^{test}_{f,g,i,j} - \nu\Sigma^{ref}_{f,g,i,j}) \end{cases} \quad (4.4)$$

The two definitions can be used to separate the error due to the 1D cross section or the reaction rate that is also affected by scattering matrices.

To minimize the manual efforts and ensure the extendibility of the tool, an HDF5 file is used to facilitate data transition and comparison. The following steps are developed to perform the analysis.

1. Print the MPACT isotopic reaction rates (group- and region-dependent) to the HDF5 output file using the internal editing routines within MPACT.
2. Convert the CE Monte Carlo (e.g., Monte Carlo N-Particle [MCNP]) output into an HDF5 file in a comparable data structure. The MPACT_MCNPconvert.py can be used with a well-defined MCNP input to generate these formatted results for MCNP. An additional file isomap.dat is required to map the isotope ZAID from MCNP to MPACT.
3. Use the MPACT_keffAnalysis.py script in the MPACT repository to analyze the two HDF5 files.

Table 4.1 lists the data compared using the reaction rate analysis tool. This tool is currently populated with MCNP results, most of which are compared for each energy group, individual isotope, and at every location, including the radial ring of the fuel.

Table 4.1. Field compared for Reaction Rate Analysis between MPACT and MCNP.

Field	By Location	By Group	By Isotope
Energy mesh	No	Yes	No
Volume	Yes	No	No
Material ID	Yes	No	No
Isotope ID	Yes	No	Yes
Number density	Yes	No	Yes
Neutron flux	Yes	Yes	No
Absorption	Yes	Yes	Yes
Nu-fission	Yes	Yes	Yes
In-scatter	Yes	Yes	Yes
Out-scatter	Yes	Yes	Yes
Self-scatter	Yes	Yes	Yes

A description of the reaction rate analysis procedure can be found in *Reaction Rate Analysis for MPACT Cross Section Library Verification* [Liu16]. While this is currently implemented for MCNP results, the process can be simplified with an extension of the VERA-Shift capability [Pan17]. This has not been included in the regular testing suite for MPACT, but it is part of the acceptance testing process when new libraries are generated.

4.5 FUTURE WORK FOR VERIFICATION DURING LIBRARY GENERATION

The verification testing that occurs during the library generation process includes several tests to ensure the quality of the final product. However, most of this verification testing is manual and is not incorporated within any regular testing program, creating the potential for changes to occur with any data/code (ENDF, AMPX, SCALE, or VERA) that might alter the final cross section library. This could have been discovered with an integrate test that indicates whether each step remains verified.

5. AUTOMATION OF THE LIBRARY GENERATION PROCESS

While each of the SCALE/AMPX, VERA/XSTools, and MPACT codes have their own SQA practices to ensure verified capabilities built upon quality software development practices, automation of the library generation process aids in ensuring that the integral product is consistently of high quality. The automation of the entire cross section process provides several quality features:

- Integrated testing of many components from multiple repositories that must work together;
- Reproducibility to ensure the elimination of all manual steps to create a production library can be recreated exactly; and
- Inherent documentation through automation of the process to allow for review and assessment.

An integrated test was established that uses the ENDF evaluations to generate an MG AMPX library using an automated process. For the initial implementation, only a small set of evaluations is selected to complete testing in a reasonable time while maintaining a representative list of nuclides for MPACT development. The selected nuclides for integrated testing are ^{1}H, ^{16}O, ^{27}Al, ^{56}Fe, ^{91}Zr, ^{234}U, ^{235}U, ^{238}U, ^{239}Pu, and ^{240}Pu. Note that this is an automation of a portion of the MG library generation process; future work is discussed in Sect. 5.3.

5.1 CONSTRAINTS OF THE AUTOMATION PROCESS

As noted in Sect. 2, the CE and MG libraries for SCALE/AMPX are generated using EXSITE to read a set of template files to generate the SCALE/AMPX inputs for individual isotopes. EXSITE requires updated infrastructure components that are not yet part of the VERA infrastructure:

- Java runtime (version $\geq$ 1.8.0), and
- CMake (version $\geq$ 3.7.0).

VERA does not currently require the Java runtime library, and the official version of CMake is 3.6.1. Therefore, additional updates to the VERA infrastructure are required before the automation process is complete, but both should be included before the release of VERA-3.8.

Currently, VERA only builds and installs a minimal set of SCALE software but no AMPX. Integration of the library generation tools within VERA will also require the following:

- build, configure, and installation of the EXSITE binary: exsite, and
- expand the SCALE data within VERA to include legacy albedos (e.g. “scale.rev00.albedos”) and weights (e.g. “scale.rev03.weights”).

5.2 IMPLEMENTATION OF AUTOMATION

The automation process is currently tested based on inputs in the regression directory of the SCALE/AMPX package. These inputs use the library.tem template file in the regression/templates/ to create a suite of inputs in the regression directory where AMPX is built.

Table 5.1. Series of Individual Tests in Automated Library Generation Advanced Test

ID	Req.	Series Names	Purpose
1		point_*	Generates 1D broadened point-wise cross section data for each isotope
2		ptab_*	Generates probability table data
3	1, 2	ce_*	Depends on pointwise (step 2) and probability table (step 3) tests
4	1, 2	neut_*	Generates MG AMPX libraries containing 1D and 2D cross section data
5	4	bond_*	Generates narrow resonance (NR) f-factors
6	4, 5	bind_*	Combines MG AMPX libraries with the Bondarenko data into NR master MG AMPX libraries
7	6	combine_nr_master	Combines the individual NR master MG AMPX libraries for each nuclide to produce a NR master library
8	7	irf_*	Generates MG libraries with lambda factors and homogenous f-factors
9	8	combine_ir_master	Combines the individual MG libraries with lambda factors and homogenous f-factors for each nuclide to produce a IR master library
10	9	irffac_U235-only	Generates MG libraries with heterogeneous f-factors for ^{235}U with single absorber model from cases listed in “U235-HetCases.inp”
11	9	irffac_Zr91-MultipleAbs	Generates MG libraries with heterogeneous f-factors for ^{91}Zr with multiple absorber model from cases listed in “scale/Zr91-HetCases.inp”
12	10, 11	compare_ir_master	Compares generated IR and NR master MG AMPX libraries
13	10	compare_U235_het_ffactors	Compares generated IR master and MG AMPX libraries with heterogeneous f-factors for ^{235}U
14	11	compare_Zr91_het_ffactors	Compares generated IR master and MG AMPX libraries with heterogeneous f-factors for ^{91}Zr
15	10	content_U235_het_ffactors	Compares selected contents MG AMPX libraries with heterogeneous f-factors for ^{235}U
16	11	content_Zr91_het_ffactors	Compares selected contents MG AMPX libraries with heterogeneous f-factors for ^{91}Zr
17	3	inf_ce_*	Runs eigenvalue problems for infinite homogenous cases with generated CE libraries
18	9	inf_mg_*	Runs eigenvalue problems for infinite homogenous cases with generated IR master MG libraries

The automation script uses an advanced TriBITS test that runs 18 individual tests, with many downstream tests that depend on proper execution of the upstream test. Test dependencies are structured so that any test will fail automatically if a dependent upstream test fails since output/results are required to successfully execute the downstream test(s). This 18-step advanced test includes each of these 19 individual tests that include ten isotopes (^{1}H, ^{16}O, ^{27}Al, ^{56}Fe, ^{91}Zr, ^{234,235,238}U, ^{239,240}Pu) at two different temperatures (293 and 800 K). The series of tests and their dependencies are shown in Table 5.1, in which * indicates that each isotope is included. Test 2, generation of the probability tables, requires the vast majority of CPU time. Tests 1–9 are

successful if they run to completion without errors, but Tests 10–18 compare the solution with a gold file to check regression.

In the current implementation, the generated CE and 252-group AMPX libraries are for testing purposes only, as they only have a limited set of nuclides and two temperatures (293 and 800 K); they should not be used for any other calculations.

5.3 ADDITIONAL AUTOMATION WORK REQUIRED

Automation of the MPACT library generation process is incomplete. Specific tasks required to fully automate the process include:

- addressing the future work required for process integration (Sect. 2.5),
- updating the third-party libraries (TPLs) and nuclear data in VERA to run EXSITE,
- creating a comprehensive automation for the CE and MG process that includes all nuclides and temperatures,
- creating a code and/or script that automates the SPH factor process, and
- expanding the 18-step SCALE/AMPX automation CTest to become a full production library generation process for all nuclides.

6. ACCEPTANCE TESTING OF NEW CROSS SECTION LIBRARIES

With continued use of MPACT for operational reactor applications and extensions to modeling new problems and code couplings, the MPACT data libraries will continue to be updated and improved. When a new library is developed using the procedure outlined within this report, a consistent set of problems will be addressed to assess the quality of the library and to determine whether to accept it for production calculations, use it for research, or reject it as flawed. The decision to accept the library for production calculations is made by the leadership within AMA based on a continually expanding suite of comparisons with operating plant data. However, the library cannot be considered ready for production by AMA until RTM has determined if it is sufficient for research and AMA testing; if there are fundamental problems with the library discovered during RTM and/or AMA testing, it is rejected for use in CASL.

Given a CE nuclear data library and a fully specified problem, Monte Carlo calculations provide the correct answer of a particular problem to within statistical uncertainty. MG deterministic transport calculations also include error that is associated with various approximations in spatial, angular, and energy discretizations. Comparison of CE Monte Carlo and MG deterministic results for a given statepoint will quantify errors in the nuclear data processing, when the spatial and angular meshes are fully refined, to verify the correct implementation. Therefore, RTM has established a suite of benchmark problems that compare CE Monte Carlo and MPACT for acceptance testing of any new library.

While CE Monte Carlo with depletion introduces discretization error (in time and space) and includes approximations in heat generation, benchmarking MPACT's use of the nuclear data library will reveal potential issues related to the depletion data and MPACT's use of it. Eight sets of benchmark suites have been developed for acceptance testing of the cross section libraries for MPACT:

[1] VERA Progression Problems [God14]
[2] Extended VERA Progression Problems [Kim17b]
[3] VERA Depletion Benchmark Problems [Kim16c]
[4] AP1000 Depletion Benchmark Problems [Gen17]
[5] Reaction Rate Analysis Problems [Liu16]
[6] Extensive PWR Pin and Assembly Benchmark Problems [Pal17a, Pal17b]
[7] BWR Assembly Benchmark Problems
[8] Non-Uniform Fuel Temperature Problems [Kim16d]

The following sections related to the benchmark calculations have results associated with the February 2017 cross section libraries in both the MPACT and SAMPX format; these are discussed in detail in *Development of the V42m5 and V5.0m0 Multigroup Cross Section Libraries for MPACT for PWR and BWR* [Kim17b]. These represent a snapshot in time of the benchmark status for a single set of libraries and are not necessarily representative of the benchmarking of previous of future libraries.

Table 6.1 provides current status of benchmark calculations by using the ENDF/B-7.0 and 7.1 MPACT and SAMPX 51 and 252-g libraries. Reference solutions have been obtained by using CE Monte Carlo codes such as CE-KENO and SHIFT developed by ORNL, MCNP developed by LANL, SERPENT developed by VTT and McCARD developed by Seoul National University (SNU). Benchmark results can be found in reference [Kim17b], and other references above. Since the benchmark suite [4] is similar to the suite [3], and the benchmark calculations for [7] are ongoing, they are not included in this report.

Table 6.1. Status for Benchmark Calculations

#	Contents	ENDF/B		Epithermal Up		MPACT		Simplified AMPX	
		7.0	7.1	No	Yes	51-g	252-g	51-g	252-g
1	VERA progression problems	X	X	X	X	X	X	X	X
2	Extended VERA progression problems	X	X	X	O	X	X	X	X
3	VERA depletion benchmark problems	X	O	X	O	X	O	Δ	O
4	AP1000 & KRSKO depletion benchmark problems	X	O	X	O	X	O	Δ	O
5	Reaction rate analysis problems	X	X	X	O	X	X	X	X
6	Extensive PWR pin & assembly benchmark problems	X	X	X	O	X	O	X	O
7	BWR pin and assembly benchmark problems	X	O	X	O	X	X	X	X
8	Nonuniform fuel temperature problems	X	O	X	O	X	O	X	O

X: Yes; O: No; Δ: Partly

6.1 VERA PROGRESSION PROBLEMS

Benchmark calculations have been performed for the VERA progression problems [God14, Kim17b] by using the MPACT and SAMPX 51- and 252-g libraries. Presently, the default cross section library for MPACT is the v4.2m5 ENDF/B-7.1 MPACT 51-g library. Recently, new SAMPX 51 and 252-g libraries have been developed which will be primary cross section libraries for MPACT in the near future after intensive testing and optimization of computational efficiency. Tables 6.2 and 6.3 provide benchmark results using the ENDF/B-7.1 MPACT 51-g and SAMPX 51 and 252-g libraries. The benchmark results are summarized as follows:

- All the MPACT and SAMPX P_2 results satisfy the accuracy goals for prediction of multiplication factors (< 200 pcm $\Delta\rho$ or Δk) and pin power distributions.
- ^{238}U epithermal upscattering resonance data (Doppler broadening rejection correction [DBRC} option in Monte Carlo) have been generated correctly.
- A temperature reactivity bias shown in the MPACT library has been almost resolved in the SAMPX library.
- Since the transport cross sections of ^{1}H have been generated to conserve neutron leakage for the whole core problems, there are some reactivity differences for single pin and assembly problems when performing transport corrected P_0 (TCP0) calculations. When using the 252-g library, the difference is much more significant.

Table 6.2. Results with the ENDF/B-7.1 MPACT 51-g Library

Up-scatt	Case	CE-KENO		MPACT P2[b]				MPACT TCP0[c]			
		k_{eff}	S.D.[a]	k_{eff}	Δk pcm	Pin power % S.D.	Pin power % Max.	k_{eff}	Δk pcm	Pin power % S.D.	Pin power % Max.
No DBRC	**1A**	**1.18698**	**0.00011**	**1.18751**	**-53**	**-**	**-**	**1.18790**	**-92**	**-**	**-**
	1B	1.18209	0.00009	1.18258	-49	-	-	1.18319	-111	-	-
	1C	1.17152	0.00008	1.17156	-4	-	-	1.17225	-73	-	-
	1D	1.16246	0.00009	1.16225	21	-	-	1.16302	-56	-	-
	1E	0.77158	0.00010	0.77311	-153	-	-	0.77289	-131	-	-
	2A	1.18191	0.00008	1.18256	-65	0.12	0.24	1.18232	-41	0.12	-0.26
	2B	1.18307	0.00009	1.18343	-37	0.12	-0.27	1.18342	-35	0.13	-0.31
	2C	1.17358	0.00010	1.17336	22	0.11	0.28	1.17340	17	0.13	0.33
	2D	1.16531	0.00010	1.16484	47	0.12	0.39	1.16495	36	0.12	0.35
	2E	1.06933	0.00009	1.06992	-59	0.13	-0.37	1.07044	-111	0.12	-0.36
	2F	0.97598	0.00009	0.97635	-38	0.15	0.40	0.97717	-119	0.15	0.39
	2G	0.84799	0.00008	0.84990	-192	0.26	0.61	0.85226	-427	0.29	0.71
	2H	0.78810	0.00012	0.78882	-72	0.22	-0.61	0.79232	-422	0.29	-0.83
	2I	1.17969	0.00008	1.18029	-60	0.13	0.31	1.18008	-39	0.14	0.29
	2J	0.97503	0.00010	0.97560	-57	0.17	-0.39	0.97641	-139	0.16	-0.39
	2K	1.01961	0.00010	1.02062	-101	0.14	0.36	1.02138	-177	0.13	0.32
	2L	1.01856	0.00010	1.01905	-49	0.12	0.33	1.01883	-27	0.13	0.34
	2M	0.93861	0.00009	0.93910	-50	0.15	-0.32	0.93881	-20	0.17	-0.43
	2N	0.86962	0.00008	0.86974	-12	0.20	0.59	0.87011	-49	0.15	0.47
	2O	1.04726	0.00010	1.04676	50	0.15	-0.37	1.04771	-45	0.16	0.37
	2P	0.92668	0.00010	0.92558	110	0.16	-0.40	0.92726	-58	0.18	-0.41
DBRC	1A	1.18603	0.00010	1.18602	1	-	-	1.18640	-37	-	-
	1B	1.18094	0.00009	1.18094	0	-	-	1.18153	-59	-	-
	1C	1.16946	0.00009	1.16900	46	-	-	1.16967	-22	-	-
	1D	1.15925	0.00009	1.15857	68	-	-	1.15932	-7	-	-
	1E	0.77099	0.00010	0.77220	-121	-	-	0.77197	-99	-	-
	2A	1.18099	0.00009	1.18122	-23	0.10	-0.28	1.18097	2	0.11	-0.29
	2B	1.18225	0.00009	1.18194	31	0.11	-0.23	1.18191	34	0.11	-0.22
	2C	1.17169	0.00008	1.17105	64	0.12	-0.27	1.17108	61	0.11	0.27
	2D	1.16252	0.00009	1.16152	100	0.10	0.31	1.16162	89	0.11	0.33
	2E	1.06840	0.00008	1.06866	-26	0.12	-0.26	1.06916	-76	0.10	-0.22
	2F	0.97501	0.00010	0.97518	-17	0.17	-0.38	0.97599	-98	0.17	-0.43
	2G	0.84716	0.00009	0.84892	-176	0.25	0.51	0.85127	-411	0.28	0.61
	2H	0.78768	0.00010	0.78793	-24	0.22	0.55	0.79142	-374	0.25	0.66
	2I	1.17858	0.00008	1.17891	-33	0.11	0.25	1.17868	-11	0.12	-0.29
	2J	0.97424	0.00009	0.97443	-19	0.13	-0.29	0.97524	-100	0.13	0.32
	2K	1.01901	0.00010	1.01941	-40	0.17	0.33	1.02016	-115	0.17	0.41
	2L	1.01774	0.00009	1.01788	-15	0.14	0.34	1.01766	8	0.16	0.38
	2M	0.93803	0.00011	0.93804	-1	0.11	-0.23	0.93774	29	0.15	-0.37
	2N	0.86882	0.00009	0.86875	8	0.17	0.42	0.86911	-29	0.13	-0.29
	2O	1.04643	0.00010	1.04555	88	0.13	-0.30	1.04649	-6	0.15	-0.39
	2P	0.92611	0.00010	0.92452	159	0.17	-0.44	0.92619	-8	0.18	-0.42

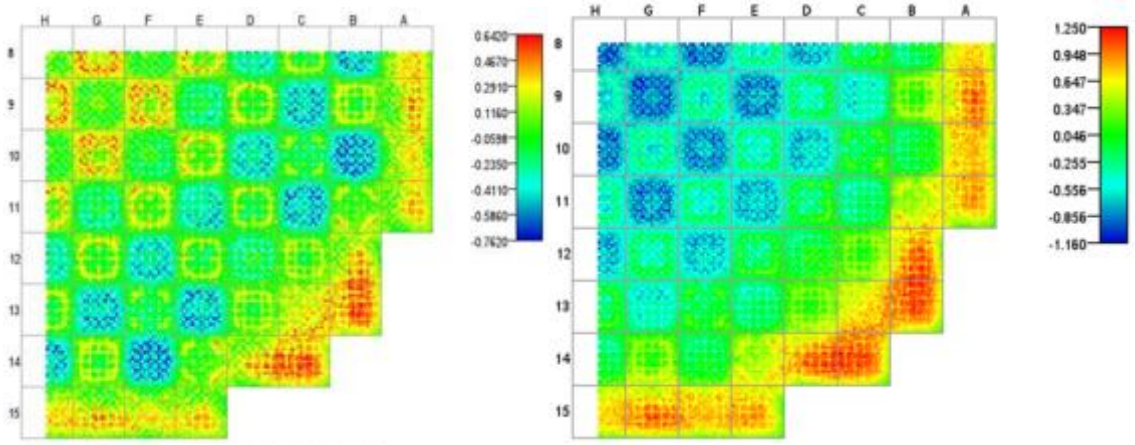
[a] S.D.: standard deviation
[b] P2: P_2 scattering
[c] TCP0: transport correct P_0 scattering

Table 6.3. Results with the ENDF/B-7.1 SAMPX 51-g Library

Up-scatt	Case	CE-KENO		SAMPX P2				SAMPX TCP0			
		k_{eff}	S.D.	k_{eff}	Δk pcm	Pin power % S.D.	Pin power % Max.	k_{eff}	Δk pcm	Pin power % S.D.	Pin power % Max.
No DBRC	1A	1.18698	0.00011	1.18727	-29	-	-	1.18771	-73	-	-
	1B	1.18209	0.00009	1.18242	-33	-	-	1.18308	-99	-	-
	1C	1.17152	0.00008	1.17165	-13	-	-	1.17240	-88	-	-
	1D	1.16246	0.00009	1.16231	15	-	-	1.16314	-68	-	-
	1E	0.77158	0.00010	0.77248	-90	-	-	0.77241	-83	-	-
	2A	1.18191	0.00008	1.18216	-26	0.12	0.24	1.18208	-17	0.12	-0.28
	2B	1.18307	0.00009	1.18312	-5	0.12	0.27	1.18326	-20	0.13	-0.32
	2C	1.17358	0.00010	1.17330	28	0.11	0.27	1.17351	7	0.13	0.32
	2D	1.16531	0.00010	1.16473	58	0.12	0.40	1.16500	31	0.12	0.34
	2E	1.06933	0.00009	1.06942	-9	0.13	-0.37	1.07019	-86	0.12	-0.34
	2F	0.97598	0.00009	0.97579	18	0.15	0.38	0.97694	-96	0.15	0.48
	2G	0.84799	0.00008	0.84983	-184	0.26	0.56	0.85275	-476	0.25	-0.61
	2H	0.78810	0.00012	0.78843	-33	0.20	-0.58	0.79268	-458	0.25	-0.73
	2I	1.17969	0.00008	1.17991	-22	0.14	0.32	1.17985	-16	0.14	0.30
	2J	0.97503	0.00010	0.97504	-1	0.16	-0.38	0.97618	-116	0.16	0.45
	2K	1.01961	0.00010	1.01992	-31	0.13	0.35	1.02099	-138	0.14	-0.32
	2L	1.01856	0.00010	1.01927	-71	0.13	0.36	1.01923	-67	0.14	-0.37
	2M	0.93861	0.00009	0.93931	-70	0.15	0.32	0.93920	-59	0.17	0.43
	2N	0.86962	0.00008	0.86975	-13	0.21	0.64	0.87042	-80	0.20	0.49
	2O	1.04726	0.00010	1.04675	51	0.16	0.37	1.04795	-69	0.15	0.39
	2P	0.92668	0.00010	0.92588	80	0.18	-0.39	0.92785	-117	0.18	-0.44
DBRC	1A	1.18603	0.00010	1.18584	19	-	-	1.18629	-26	-	-
	1B	1.18094	0.00009	1.18085	8	-	-	1.18152	-59	-	-
	1C	1.16946	0.00009	1.16889	57	-	-	1.16965	-19	-	-
	1D	1.15925	0.00009	1.15885	40	-	-	1.15969	-44	-	-
	1E	0.77099	0.00010	0.77161	-62	-	-	0.77155	-56	-	-
	2A	1.18099	0.00009	1.18087	12	0.11	-0.27	1.18079	20	0.11	-0.30
	2B	1.18225	0.00009	1.18169	56	0.11	-0.22	1.18184	40	0.11	-0.25
	2C	1.17169	0.00008	1.17077	92	0.12	-0.27	1.17100	70	0.11	0.27
	2D	1.16252	0.00009	1.16159	92	0.10	0.31	1.16188	64	0.11	0.33
	2E	1.06840	0.00008	1.06820	20	0.12	-0.26	1.06899	-58	0.11	-0.26
	2F	0.97501	0.00010	0.97467	34	0.17	-0.37	0.97582	-81	0.17	0.50
	2G	0.84716	0.00009	0.84889	-173	0.24	0.49	0.85182	-466	0.24	-0.60
	2H	0.78768	0.00010	0.78760	8	0.19	0.55	0.79185	-417	0.23	0.47
	2I	1.17858	0.00008	1.17857	0	0.11	0.25	1.17852	5	0.13	-0.31
	2J	0.97424	0.00009	0.97392	32	0.13	0.28	0.97507	-83	0.15	0.34
	2K	1.01901	0.00010	1.01875	26	0.17	0.35	1.01983	-82	0.17	0.51
	2L	1.01774	0.00009	1.01814	-41	0.15	-0.35	1.01812	-38	0.16	0.40
	2M	0.93803	0.00011	0.93829	-26	0.12	-0.24	0.93819	-16	0.16	-0.42
	2N	0.86882	0.00009	0.86879	3	0.18	0.41	0.86947	-65	0.19	-0.52
	2O	1.04643	0.00010	1.04558	85	0.14	-0.3	1.04679	-36	0.15	-0.37
	2P	0.92611	0.00010	0.92486	125	0.19	-0.45	0.92684	-73	0.20	0.43

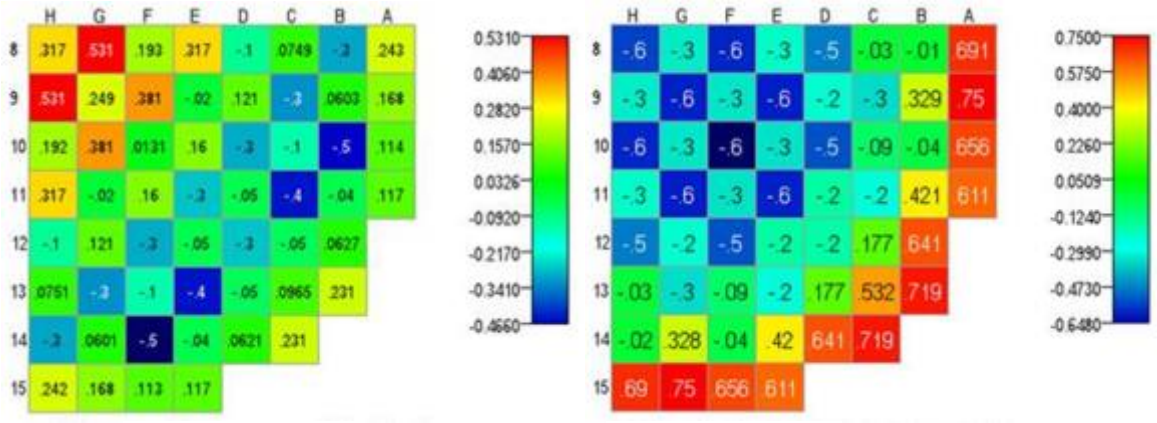
Table 6.4. Results for 5A with the ENDF/B-7.0 Library

Problem	Parameter	MPACT	SAMPX
5A-2D	Δk diff. (pcm)	44	11
	Radial power, RMS (%)	0.262	0.552
	Radial power, Max. (%)	0.762	1.249
5A-3D	Δk diff. (pcm)	45	15
	3D pin power, RMS (%)	0.468	0.644
	3D pin power, Max. (%)	2.688	2.777
	Axial power, RMS (%)	0.276	0.286
	Axial power, Max. (%)	0.459	0.460
	Axial power, Axial Offset (%)	0.242	0.243
	Radial power, RMS (%)	0.270	0.486
	Radial power, Max. (%)	0.818	1.112
	3D Assembly power, RMS (%)	0.391	0.585
	3D Assembly power, Max. (%)	1.157	1.367
	2D Assembly power, RMS (%)	0.237	0.463
	2D Assembly power, Max. (%)	0.531	0.750



(a) MPACT library (b) SAMPX library

Figure 6.1. Pin Power Comparisons for Problem 5A-2D.



(a) MPACT library (b) SAMPX library

Figure 6.2. Assembly Power Comparisons for Problem 5A-3D.

- Cases 2G and 2H are control rod insertion cases which show significant k_{eff} differences when performing TCP0 calculations. The TCP0 calculation is not able to correctly simulate highly anisotropic neutron angular fluxes in and around control Rods are in single-lattice rodded problems, but these errors dissipate in full-core calculations.
- Prediction of the power distribution is good for all cases regardless of the number of energy groups.

Table 6.4 and Figures 6.1 and 6.2 provide benchmark results for the VERA progression problem 5A's 2D and 3D quarter core problems by using the v4.2m5 MPACT and v5.0m0 SAMPX 51-g libraries. The reference solutions were obtained by using CE-KENO with the ENDF/B-7.0 nuclear data. The benchmark results with the v4.2m5 MPACT and v5.0m0 SAMPX 51-g libraries with ENDF/B-7.0 are very consistent with the reference CE-KENO result for both multiplication factor and pin power distributions. The SAMPX library result for multiplication factor is better than the MPACT library results. However, the MPACT library results for radial and axial pin and assembly power distributions are slightly better than the SAMPX library results.

6.2 EXTENDED VERA PROGRESSION PROBLEMS

Since the VERA core physics benchmark progression problems do not include various ^{235}U enrichment and burnup compositions, additional benchmark problems were developed to determine the sensitivities of the libraries to ^{235}U enrichment, burnup, and the number of radial fuel rings [Kim17b]. These benchmark problems are based on VERA progression problems 1B and 1C. Cases 1C-10-1h through 1C-60-1h include only heavy nuclides, excluding fission product isotopes. Benchmark calculations have been performed using the ENDF/B-7.0 and 7.1 MPACT and SAMPX 51-g libraries. The benchmark results are provided in Tables 6.5 and 6.6.

Table 6.5. Benchmark Result with the ENDF/B-7.1 MPACT 51-g Library

Case	No Epithermal Upscatt			Epithermal Upscatt		
	KENO	P2, pcm	TCP0, pcm	KENO	P2, pcm	TCP0, pcm
1C-21	1.07008	-46	-86	1.06908	7	-32
1C-26	1.13506	-69	-114	1.13402	-13	-57
1C-31	1.18199	-59	-109	1.18087	-7	-54
1C-36	1.22098	-58	-111	1.21992	4	-47
1C-41	1.25239	-75	-131	1.25153	9	-45
1C-46	1.27881	-51	-109	1.27764	4	-53
1C-00-3a	1.24699	48	-25	1.24496	111	40
1C-10-3a	1.08728	-86	-169	1.08541	-65	-147
1C-20-3a	1.00259	-45	-164	1.00111	-6	-125
1C-40-3a	0.88304	34	-111	0.88157	47	-97
1C-60-3a	0.80899	22	-127	0.80736	2	-147
1C-10-1h	1.17408	-11	-101	1.17176	-14	-103
1C-20-1h	1.11658	81	-50	1.11468	106	-25
1C-40-1h	1.03617	186	21	1.03419	186	23
1C-60-1h	0.98862	228	56	0.98682	236	65

Table 6.6. Benchmark Result with the v5.0m0 ENDF/B-7.1 SAMPX 51-g Library

Case	No Epithermal Upscatt			Epithermal Upscatt		
	KENO	P2, pcm	TCP0, pcm	KENO	P2, pcm	TCP0, pcm
1C-21	1.07008	-35	-93	1.06908	10	-50
1C-26	1.13506	-54	-117	1.13402	-6	-70
1C-31	1.18199	-43	-109	1.18087	2	-65
1C-36	1.22098	-38	-107	1.21992	16	-55
1C-41	1.25239	-53	-125	1.25153	24	-50
1C-46	1.27881	-27	-102	1.27764	20	-57
1C-00-3a	1.24699	16	-73	1.24496	101	10
1C-10-3a	1.08728	-114	-215	1.08541	-56	-158
1C-20-3a	1.00259	-143	-280	1.00111	-67	-205
1C-40-3a	0.88304	-95	-259	0.88157	-48	-212
1C-60-3a	0.80899	-133	-302	0.80736	-120	-290
1C-10-1h	1.17408	-93	-201	1.17176	-55	-164
1C-20-1h	1.11658	-86	-234	1.11468	-19	-168
1C-40-1h	1.03617	-19	-198	1.03419	23	-158
1C-60-1h	0.98862	21	-165	0.98682	70	-117

6.3 VERA DEPLETION BENCHMARK PROBLEMS

The VERA depletion benchmark problems [Kim16c] were developed based on the VERA progression problems [God14]. The depletion benchmark suite includes 9 single pin and 16 fuel assembly problems with various fuel temperatures, ^{235}U enrichments, control rods, and burnable poisons. The benchmark calculations were performed using VERA-CS (MPACT+ORIGEN) with the ENDF/B-7.0 MPACT and SAMPX 51-g libraries, with simplified and full burnup chains. Reference solutions have been obtained by using two CE Monte Carlo codes—SERPENT and McCARD—using ENDF/B-7.0 data. Since multiplication factors as a function of burnup are sensitive to neutron flux levels, the same values of recoverable energies per fission have been used for all three codes [Kim16c]. Figures 6.3–6.5 provide comparisons of multiplication factors as a function of burnup for representative cases including fuel assemblies with UO_2 fuels, WABA+IFBA burnable poisons and gadolinium rods. The VERA-CS results with the MPACT and SAMPX 51-g libraries are very consistent with the SERPENT and McCARD results, within 100 pcm at all burnup points.

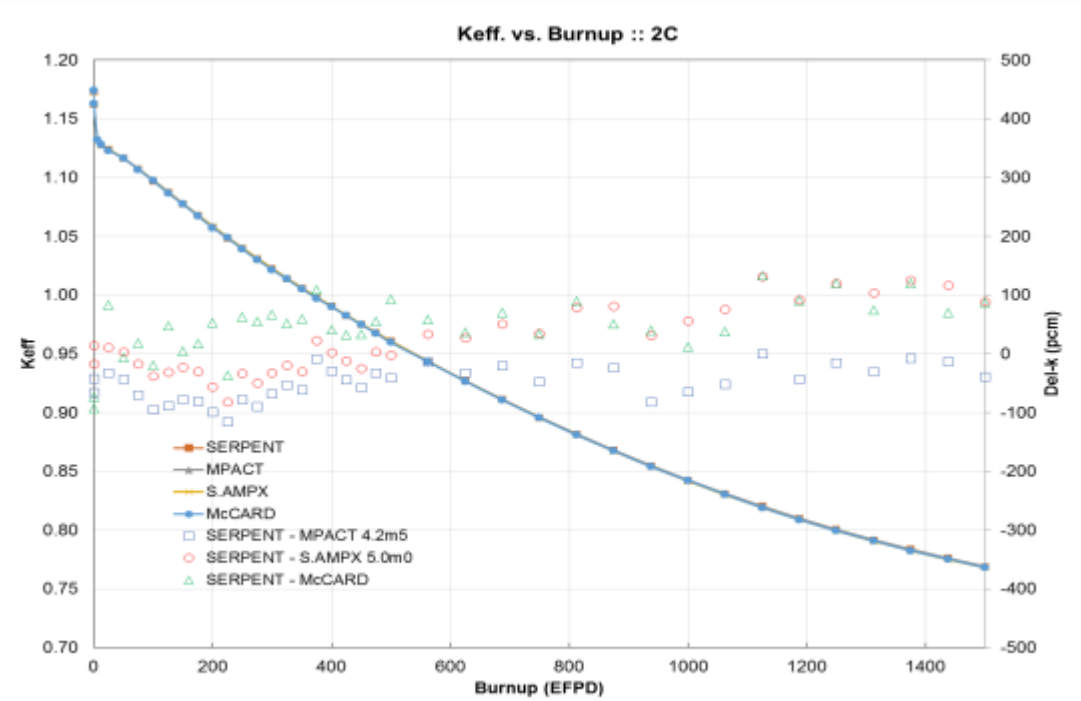


Figure 6.3. Comparison of Multiplication Factors for Case 2C.

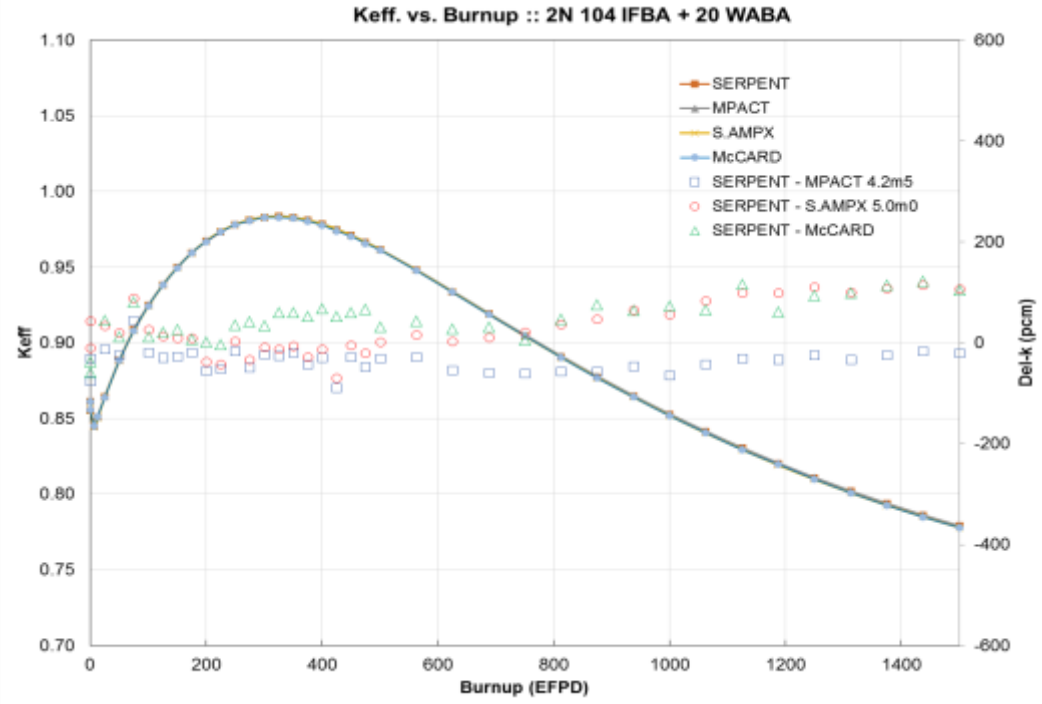


Figure 6.4. Comparison of Multiplication Factors for Case 2N.

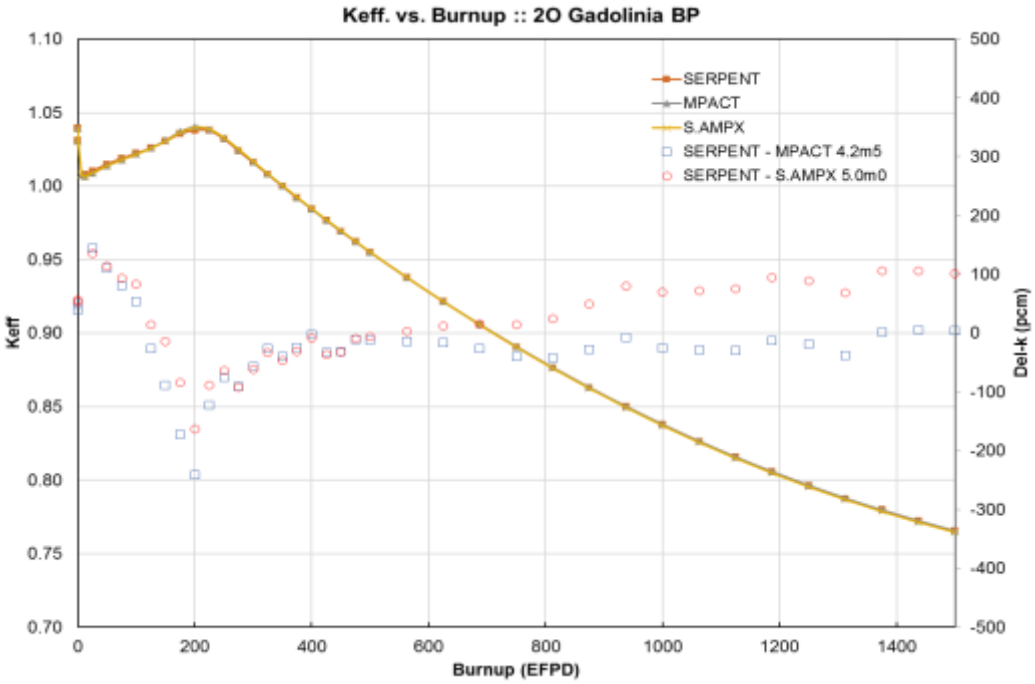


Figure 6.5. Comparison of Multiplication Factors for Case 2O.

6.4 REACTION RATE ANALYSIS PROBLEMS

Eighteen representative cases were developed for reaction rate analysis, as described in Sect. 5.4, with various ^{235}U enrichments, fuel and moderator temperatures, soluble boron concentrations, burnup and void fractions for both PWR and BWR. Currently, reference solutions were obtained by MCNP with ENDF/B-7.0 and 7.1. A more detailed description can be found in *Reaction Rate Analysis for MPACT Cross Section Library Verification* [Liu16].

Tables 6.7 and 6.8 provide reaction rate analysis by using the ENDF/B-7.1 MPACT and SAMPX 51-g libraries. There are error cancellations between absorption and ν*fission reactions in ^{235}U at thermal energy groups. This may be an intrinsic issue shown in coarse group approximation due to poor thermal scattering matrices. BWR cases show relatively large reaction rate differences compared to PWR cases since resonance data have been generated and optimized for PWR fuel configuration. The issue can be partly resolved by generating ^{238}U resonance data based on the BWR geometry. Errors in the 51-group structure for high-void BWR cases are larger than the target; the energy group structure may need to be refined to capture the harder spectra compared to the typical PWR. Fuel temperature reactivity bias is seen when comparing Cases 5(600K), 1(900K) and 6(1200K). The MPACT and SAMPX MG libraries were generated by using the SCALE/AMPX code packages by which SCALE-KENO shows intrinsic difference in fuel temperature coefficients compared to MCNP.

Table 6.7. Analysis Result for the ENDF/B-7.1 MPACT 51-g Library

No	Case	k_{eff}		Δk, pcm		Absorption, pcm			ν*Fission, pcm		
		MCNP[a]	MPACT[b]	[a-b]	RR	Nuclide	Δk	Δk (grp)	Nuclide	Δk	Δk (grp)
1	rr_1_3.1%	1.29874	1.29762	-112	-113	922380	-112	-142.0(23)	922380	-13	-6.3(2)
2	rr_2_2.1%	1.21266	1.21155	-111	-121	922380	-126	-146.0(23)	922350	-35	127.4(45)
3	rr_3_4.1%	1.34863	1.34771	-92	-88	922380	-80	-132.6(23)	922380	-15	-6.3(2)
4	rr_4_293.6K	1.39603	1.39556	-47	-49	10010	112	62.1(50)	922380	-38	-17.5(4)
5	rr_5_600K	1.31010	1.31015	5	9	922350	-71	104.6(43)	922350	88	-155.0(43)
6	rr_6_1200K	1.28892	1.28706	-187	-184	922380	-165	-153.3(23)	922350	-76	-161.7(43)
7	rr_7_B600	1.23711	1.23678	-33	-47	922380	-94	-125.8(23)	922350	50	-157.8(43)
8	rr_8_B1300	1.17364	1.17372	8	14	922380	-95	-119.5(23)	922350	136	-152.3(43)
9	rr_9_bwr_0	1.37369	1.37121	-248	-246	922380	-287	-146.1(23)	922350	-17	-178.8(43)
10	rr_10_bwr_50	1.22621	1.22407	-215	-212	922350	239	145.4(43)	922350	-399	-229.8(43)
11	rr_11_bwr_70	1.10150	1.10064	-86	-89	922350	321	131.6(43)	922350	-546	-231.2(43)
12	rr_12_bwr_90	0.88894	0.89091	197	188	922380	432	190.5(14)	922350	-775	-135.9(43)
13	rr_13_burn_0	1.24743	1.24690	-53	-36	922380	-111	-133.0(23)	922350	97	-144.1(43)
14	rr_14_burn_001	1.20383	1.20367	-16	-14	922380	-97	-120.5(23)	922350	99	-146.8(43)
15	rr_15_burn_20	1.00246	1.00286	40	35	942390	206	85.8(43)	942390	-309	-143.3(43)
16	rr_16_burn_40	0.88270	0.88265	-5	-17	942390	144	62.8(43)	942390	-244	-119.0(43)
17	rr_17_burn_60	0.80859	0.80880	21	15	942390	125	52.1(43)	942390	-236	-107.8(43)
18	rr_18_erbium	1.01241	1.01100	-141	-147	922380	-87	-100.9(23)	922350	-56	-126.8(43)

Table 6.8. Analysis Result for the ENDF/B-7.1 SAMPX 51-g Library

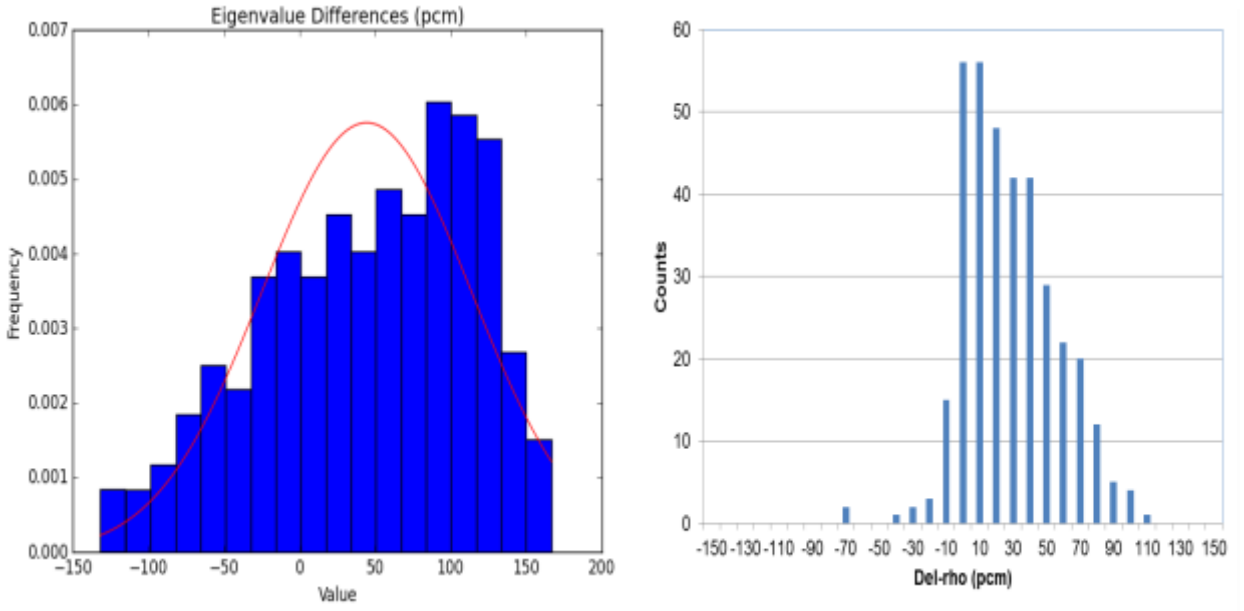
Case	k_{eff}		Δk, pcm		Absorption, pcm			ν*Fission, pcm		
	MCNP[a]	MPACT[b]	[a-b]	RR	Nuclide	Δk	Δk (grp)	Nuclide	Δk	Δk (grp)
rr_1_3.1%	1.29874	1.29775	-99	-100	922380	-57	-116.3(23)	922380	-18	-14.6(3)
rr_2_2.1%	1.21266	1.21167	-99	-110	922380	-80	-121.7(23)	922350	-32	-137.1(50)
rr_3_4.1%	1.34863	1.34785	-78	-74	922350	-29	96.2(43)	922380	-20	-14.2(3)
rr_4_293.6K	1.39603	1.39531	-72	-75	10010	76	51.9(50)	922380	-42	-19.8(3)
rr_5_600K	1.31010	1.31000	-10	-6	922350	-78	78.6(43)	922350	72	-120.0(43)
rr_6_1200K	1.28892	1.28716	-176	-174	922380	-112	-131.6(23)	922350	-73	-125.7(43)
rr_7_B600	1.23711	1.23675	-36	-50	922350	-59	76.8(43)	922350	45	-123.6(43)
rr_8_B1300	1.17364	1.17355	-10	-3	922350	-99	71.1(43)	922350	123	-120.4(43)
rr_9_bwr_0	1.37369	1.37081	-288	-287	922380	-263	-124.1(23)	922350	-83	-139.4(43)
rr_10_bwr_50	1.22621	1.22400	-221	-218	922350	210	115.9(43)	922350	-381	-187.3(43)
rr_11_bwr_70	1.10150	1.10080	-70	-74	922350	272	105.3(43)	922350	-485	-189.2(43)
rr_12_bwr_90	0.88894	0.89180	286	276	922380	338	163.8(14)	922350	-617	-104.4(43)
rr_13_burn_0	1.24743	1.24695	-48	-31	922350	-85	69.6(43)	922350	90	-111.3(43)
rr_14_burn_001	1.20383	1.20377	-6	-4	922350	-68	70.1(43)	922350	69	-115.9(43)
rr_15_burn_20	1.00246	1.00360	114	110	942390	169	80.5(43)	922350	328	89.7(45)
rr_16_burn_40	0.88270	0.88362	92	80	922350	-70	-18.9(45)	922350	166	46.4(45)
rr_17_burn_60	0.80859	0.80998	139	134	922380	83	-67.2(23)	922350	67	21.5(45)
rr_18_erbium	1.01241	1.01066	-175	-181	681670	-95	-81.0(41)	922350	-80	-102.8(43)

6.5 EXTENSIVE PWR PIN AND ASSEMBLY BENCHMARK PROBLEMS

Extensive benchmark problems for PWR fuel pins and fuel assemblies were developed to determine how well the MPACT MG library agrees with CE Monte Carlo results [Pal17a, Pal17b]. There is a total of 360 cases, 324 (3 × 4 × 3 × 3 × 3) hot cases, and 36 (3 × 4 × 3) cold cases. The PWR fuel pin cases consist of three ^{235}U enrichments, four rod sizes, three hot coolant densities, three hot fuel temperatures, cold cases at room temperature, and three boron concentrations. Additional benchmark problems have been developed for fourteen different PWR assembly types, including 15 × 15, 16 × 16, and 17 × 17 designs by different fuel vendors, with many different state point conditions encountered in a reactor. There is a total of 81 hot cases (3 × 3 × 3 × 3) and 9 cold cases (3 × 3) per assembly, for a total of 1,260 cases. Each assembly type includes 90 different state points. Benchmark calculations by the ENDF/B-7.0 MPACT 51-g and ENDF/B-7.1 SAMPX 51-g libraries are summarized [Pal17a, Pal17b].

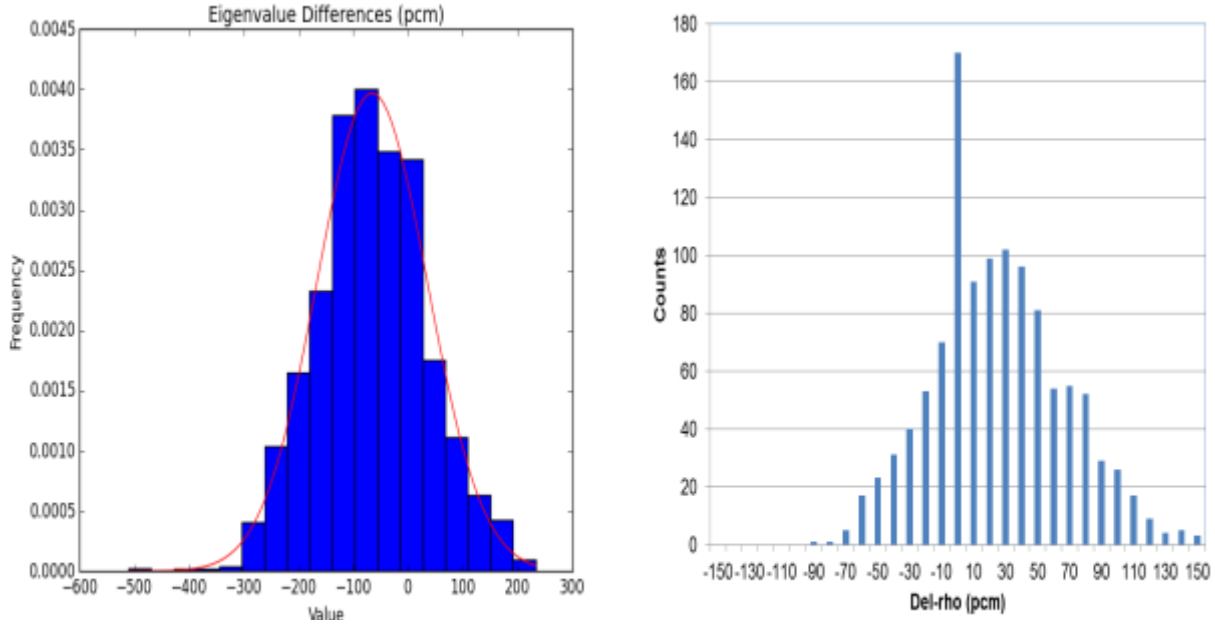
Figure 6.6 presents a summary in a histogram of the PWR pin cell eigenvalue results for MPACT with the ENDF/B-7.0 v4.2m5 MPACT 51-g library and MCNP and CE_KENO with ENDF/B VII.0. The left-hand side in Figure 6.6 shows the differences between the MCNP and MPACT eigenvalues in pcm. Overall, the PWR pin results are acceptable. The average of all 324 hot cases was 50 pcm with a standard deviation of 67 pcm. All the hot cases were between -132 and +167 pcm. The cold cases had an approximately -58 pcm bias compared with the hot cases. The right-hand side of the figure shows the reactivity differences between the CE-KENO and MPACT eigenvalues in pcm. The differences are much less than those between MCNP and MPACT due to the different fuel temperature coefficients between MCNP and CE-KENO.

Figure 6.7 presents a summary of PWR assembly benchmark results in a histogram. Overall, the eigenvalue results compared to the MCNP results are acceptable. The average of all 1,134 hot cases is -72 pcm with a standard deviation of 94 pcm. All the hot cases are between -277 and +184 pcm. A reasonable goal is to have all eigenvalue differences between +/- 200 pcm. The cold cases have a bias of approximately +60 pcm compared to the hot cases, and a larger standard deviation. The hot pin power results look very good. All the hot assemblies have a maximum pin power of less than 0.5%. The cold pin power results are not as good, with maximum error of almost 1%. It is suspected that additional coolant rings should be included in the cold cases to reduce the maximum pin power errors. In addition, the reference solutions were obtained by the CE-KENO calculations for hot zero and full power cases, and the MPACT calculations were performed again by using the ENDF/B-7.0 v4.2m5 MPACT 51-g library with improved resonance data for ^{155}Gd and ^{157}Gd. The results were significantly improved to have all hot cases between -100 and 150 pcm.



MCNP vs. MPACT KENO vs. MPACT

Figure 6.6. Pin k_{eff} Difference Distribution with the v4.2m5 ENDF/B-7.0 MPACT 51-g Library.



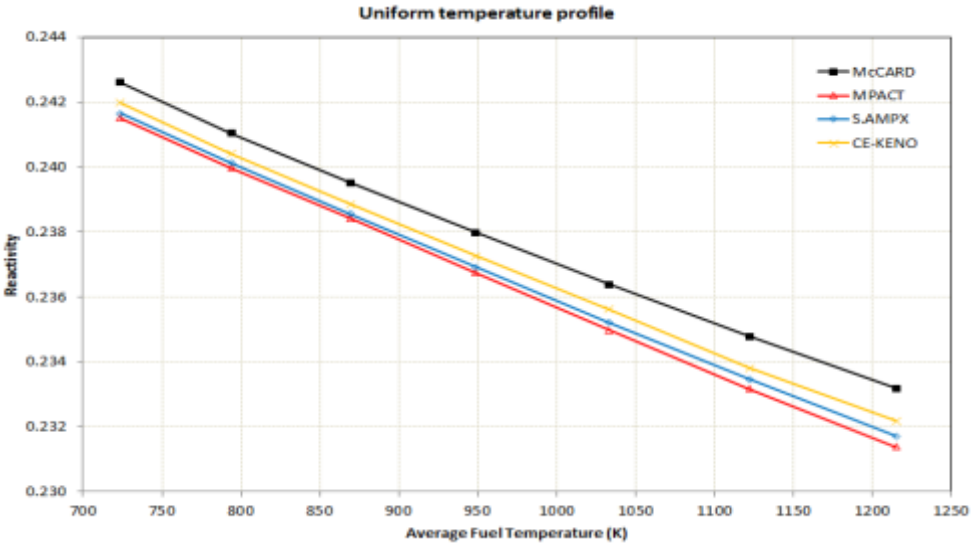
MCNP vs. MPACT KENO vs. MPACT

Figure 6.7. Assembly k_{eff} Difference Distribution with the v4.2m5 ENDF/B-7.0 MPACT 51-g Library.

6.6 NONUNIFORM FUEL TEMPERATURE BENCHMARK PROBLEMS

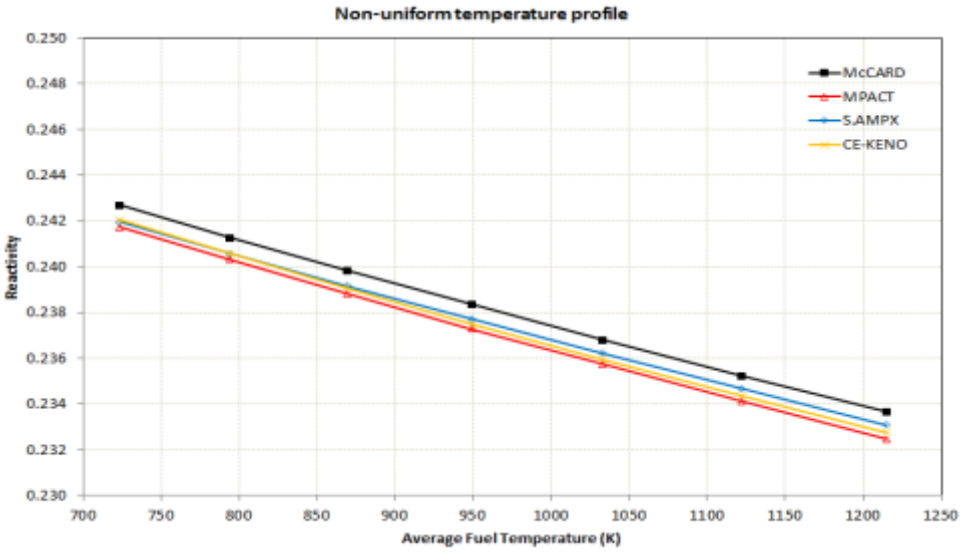
SNU has developed a benchmark suite for the intra-pellet nonuniform temperature distribution cases [Kim16d]. Benchmark calculations were performed using the CE Monte Carlo codes McCARD and CE-KENO using the ENDF/B-7.0 CE cross section library and VERA-CS MPACT using the ENDF/B-7.0 MPACT and SAMPX 51-g libraries. The ACE format CE cross sections for McCARD were processed for all temperatures by NJOY [Mac94]. SCALE-6.2 with CE-KENO includes a new capability to interpolate CE cross sections for any specified temperature based on the reference temperatures for base cross sections. However, if the specified temperature differs from the reference temperature within 4 K, no interpolation will be made.

Figure 6.8 presents the benchmark results for the uniform temperature cases. There is very good agreement between KENO and MPACT with the MPACT and SAMPX libraries in the reactivities for all temperatures. While the difference in fuel temperature coefficient is about 3% between KENO and MPACT with the MPACT library, very good agreement can be observed between KENO and MPACT with the SAMPX 51-g library. It should be noted that there is an intrinsic difference in reactivity between McCARD and KENO. McCARD is using the ACE format library and is almost identical to MCNP in methodology.



Code	FTC (pcm/K)	[a]-[b,c] (%)	[b]-[a,c](%)
McCARD[a]	-1.934	-	-3.6
CE-KENO[b]	-2.004	3.5	-
SAMPX[c]	-2.032	4.8	1.3
MPACT[c]	-2.068	6.4	3.1

Figure 6.8. Comparison of Reactivities for the Uniform Temperature Distributions.



Code	FTC (pcm/K)	[a]-[b,c] (%)	[b]-[a,c](%)
McCARD[a]	-1.847	-	-2.8
CE-KENO[b]	-1.899	2.7	-
S.AMPX[c]	-1.933	-2.0	-4.9
MPACT[c]	-1.788	-2.5	-0.2

Figure 6.9. Comparison of Reactivities for the Nonuniform Temperature Distributions.

Figure 6.9 provides the benchmark results for the nonuniform temperature cases. There is very good agreement between KENO and MPACT, with the MPACT and SAMPX libraries in the reactivities for all temperatures. However, while there is about 5% difference in fuel temperature coefficient between KENO and MPACT with the SAMPX library, very good agreement can be observed between KENO and MPACT with the MPACT 51-g library. There is intrinsic difference in reactivity between McCARD and KENO.

6.7 EVALUATION OF RESULTS FOR DETERMINATION OF ACCEPTANCE

The benchmark problems do not provide a direct pass-fail result. These results are compiled for each library, and a collective of key stakeholders discusses the results and makes a final determination. For example, there were 6 versions of the MPACT 51-group ENDF/B-VII.1 library generated between August and December 2016. While major changes from the previous production library (e.g., from 47 groups to 51) were embedded in the first version, there were many relatively minor changes that occurred in each of the subsequent five modifications. When all key stakeholders were satisfied with the comparisons of MPACT and CE Monte Carlo for all benchmark problems, the modification 5 version of the 51-group library was released in VERA-3.6 after being accepted by RTM for use by AMA and by AMA for production analyses.

6.8 FUTURE WORK RELATED TO ACCEPTANCE TESTING

The acceptance testing process is slowed down significantly by the breadth of Monte Carlo codes used. Significant duplication in each these benchmark (many pin cells in

benchmark suites are nearly identical), providing a false-positive level of confidence in the breadth of applicability of the results. In addition, differences between Monte Carlo codes can be significant for many reasons, leading to significant confusion during acceptance testing discussions. Based on these concerns, there are significant benefits to using Shift as the primary Monte Carlo code for comparison with MPACT data libraries:

- Shift, CE-KENO, and MPACT use data libraries generated from identical CE nuclear data, eliminating differences in CE data between NJOY and AMPX as a source of confusion.
- Shift and MPACT can be executed from a single input using VERA-Shift to run VERA, then Shift, for each statepoint in the problem, thus eliminating the need for significant post-processing of output files.
- Shift is massively parallel, thus ensuring that very few problems for which an MPACT comparison is desired can be executed.

Future work related to acceptance testing should include the following objectives:

- Enhance Shift and VERA-Shift capability for resonance upscattering, reaction rates comparisons, and depletion.
- Independently review and assess Shift verification and validation (V&V) to qualify it for use as the primary tool for acceptance testing.
- Generate benchmark results from Shift for each of these problems, and populate required acceptance testing gold files.
- Incorporate each benchmark evaluation as part of the VERA-Shift testing suite, even if only run on an occasional basis.

7. CONCLUSIONS AND FUTURE WORK

This report documents the current status of the software quality, verification, and acceptance testing of nuclear data libraries for MPACT. It provides a brief overview of the library generation process: from general-purpose ENDF/B to a subgroup library for modeling LWRs. The SQA programs, including the software used to generate the nuclear data libraries, are discussed, and specific tests within the SCALE/AMPX and VERA/XSTools repositories are described. The methods and associated tests required to verify the quality of the library during the generation process are described in detail. The library generation process has been automated to a degree to ensure (1) that it can be run without user intervention, and (2) to ensure that the library can be reproduced. Finally, the acceptance testing process to be performed by representatives from the RTM Focus Area prior to the production library's release is described in detail.

The software quality for the library generation process has improved significantly over the past 18 months. Several independent evaluations of the AMPX SCALE/AMPX and VERA portions of the process were a primary mechanism for this improvement. These evaluations (1) enhanced knowledge transfer among technical staff members (2) increased mutual understanding of the status and capability of each software component, and (3) guided the development of improvements. During this process, all software was included in an ORNL SQA program. Unit and/or regression tests were established for each package, and many software bugs were fixed. The library generation process was automated to ensure integrated testing of all components, as well as reproducibility of the final product. Automation also provided an ingrained level of inherent documentation.

As the quality of the library generation process improved, the rigor of acceptance testing increased. A suite of eight comparisons of MPACT results with CE Monte Carlo solutions provides a clear basis for identifying errant data or data trends that reveal discrepancies in the final library. CASL stakeholders can review these comparisons and see the benefits of a given library compared to previous versions. This establishes a clear pathway from library development to application within VERA and eventual release with MPACT.

However, many important objectives remain to improve the quality of the library generation process. Section 2.5 notes the following future work activities related to the library generation process:

- Extension of AMPX to read the fission κ values from ENDF/B;
- Extension of AMPX to estimate the KERMA factors to add the capture κ values;
- Extension of AMPX to generate the time-dependent data;
- Implementation of resonance upscatter in AMPX using CE-KENO or CENTRM;
- Additional unit and verification tests of SUBGR;
- Extension of heterogeneous IRFFACTOR to read external resonance cross section tables to enable; and
- Creation of a VERA library generation process that calls SCALE/AMPX and MPACT to generate the full MG cross section library with subgroup data, resonance upscattering, and SPH factors.

Section 3.4 notes the following future work activities related to the SQA of the library generation process:

- Deprecation of the Moc1D and FF2RI packages, as they will no longer be used;
- Enhancement of IRFFACTOR with KENO and/or Shift to compute background cross sections for resonance upscattering and the SPH factors so that MERIT can be deprecated;
- Substantial increase in the unit testing of routines in DecLib;
- Incorporation of supplemental data into the MG AMPX library so the SAMPX library can be generated automatically by VERA with SCALE/AMPX; and
- Direct use of the MG AMPX library in MPACT to eliminate need for SAMPX.

Section 4.5 notes that most of the verification tests are not automated, thus allowing for the results presented in Section 4 to be simply a snapshot in time that is no longer valid.

Section 5.3 notes the additional work required for automation of the library generation process:

- Update of the TPLs and nuclear data in VERA to run EXSITE;
- Creation of a comprehensive automation for the CE and MG process that includes all nuclides and temperatures;
- Creation of a code and/or script that automates the SPH factor process; and
- Expansion of the 19-step SCALE/AMPX automation CTest to become a full production library generation process for all nuclides.

Section 6.8 notes the benefits of identifying Shift as the primary Monte Carlo code for MPACT library benchmarking and specifically acknowledges the following action items:

- Enhance Shift, and VERA-Shift, capability for resonance upscatter, reaction rates comparisons, and depletion;
- Independently review and assess Shift V&V to qualify it for use as the primary tool for acceptance testing;
- Generate benchmark results from Shift for each of these problems and populate required acceptance testing gold files; and
- Incorporate each of these benchmark evaluations as part of the VERA-Shift testing suite, even if only run on an occasional basis.

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