

DEVELOPMENT OF THE MPACT 69-GROUP LIBRARY FOR MAGNOX REACTOR ANALYSIS USING CASL VERA

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ABSTRACT

The Consortium for Advanced Simulation of Light Water Reactors (CASL) has developed the CASL toolset, Virtual Environment for Reactor Analysis (VERA), for pressurized water reactor (PWR) analysis. Recently the CASL VERA was improved for Magnox reactor analysis, which required the development of a new cross section library and new geometrical and thermal feedback capabilities for graphite-moderated Magnox reactors. The MPACT neutronics module of the CASL core simulator is a 3D whole core transport code, which requires a new cross section library with a different energy group structure due to the different neutronic characteristics of Magnox compared with PWR. A new 69-group structure was developed based on the MPACT 51-group structure to have more thermal energy groups and to be a subset of the SCALE 252-group structure. The ENDF/B-VII.1 MPACT 69-group library was developed for Magnox reactor analysis using the SCALE/AMPX and VERA-XSTools for which a super-homogenization method was applied, and transport cross sections were generated for graphite using a neutron leakage conservation method. Benchmark results show that new MPACT 69-group library works reasonably well for Magnox reactor analysis.

KEYWORDS: Magnox, VERA MPACT, cross section library

1. INTRODUCTION

The MPACT neutronics module [1] of the Consortium for Advanced Simulation of Light Water Reactors (CASL) [2] core simulator is a 3D whole core transport code being developed for the CASL toolset, Virtual Environment for Reactor Analysis (VERA) [3]. MPACT has been developed for neutronics and thermal-hydraulics coupled simulation for light water reactors (LWR) and is recently being improved to apply for various reactor analyses such as molten salt and graphite-moderated reactor systems. Key characteristics of the MPACT code include (1) a subgroup method for resonance self-shielding and (2) a whole core solver with a 1D/2D synthesis method [4]. Oak Ridge National Laboratory (ORNL) AMPX/SCALE code packages [5] have been significantly improved to support various intermediate resonance self-shielding approximations such as subgroup [6] and embedded self-shielding methods [7]. The ENDF/B VII.0, VII.1 and VIII.0 MPACT 51-group libraries [8] were successfully developed for the CASL neutronics module MPACT for LWR analysis. The 51-group structure was optimized to perform LWR analysis with minimizing computing time and memory. Additionally, special transport cross sections for ¹H were generated using a neutron leakage conservation (NLC) method [10] for the transport-corrected P₀

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calculation to significantly save computing time without losing accuracy, and equivalence parameters called super-homogenization (SPH) factors were applied to conserve reaction rates at resonance groups.

However, these MPACT 51-group libraries cannot be used for Magnox reactor [11] analysis because neutron spectra of Magnox are very different from and much softer than the spectra of LWRs due to the graphite moderator. A new 69-group structure was developed, special transport cross sections for graphite were generated using the NLC method, and an improved SPH procedure was applied to ^{238}U self-shielded cross section tables to conserve reaction rates at both thermal and resonance energy groups with which the ENDF/B-VII.1 MPACT 69-group library was developed for Magnox reactor analysis. The MPACT 69-group library has been verified by performing reaction rate analysis, benchmark calculations, and a code-to-code comparison with continuous energy Monte Carlo results. A companion paper demonstrates more detailed benchmark results to verify the MPACT 69-group library [12].

2. DEVELOPMENT OF THE MPACT 69-GROUP LIBRARY

2.1 Neutronic Characteristics of Magnox Fuel

Magnox reactors [10] were made to produce electrical power and ^{239}Pu . The use of graphite as a moderator allows Magnox reactors to run with natural uranium while other LWRs use enriched uranium. Figure 1 compares neutron spectra at the SCALE 252-group structure between Magnox and PWR reactors. The Magnox neutron spectrum is very softened and includes a thermal peak around 0.15 eV, which is much bigger than the PWR thermal peak. Diffusion lengths of the graphite-moderated fuel and reflector are about 3 and 14 times longer than the diffusion lengths of the PWR fuel and reflector, respectively. [13] The VERA MPACT has successfully used the MPACT 51-group library for PWR analysis. However, these Magnox neutronic characteristics would require more thermal energy groups due to a much higher thermal peak and significant environmental influence caused by very long diffusion lengths. Therefore, since thermal reaction rates are dominant in core reactivity and local neutron spectra are significantly influenced by surrounding materials, a new energy group structure needs to be developed for Magnox reactor analysis.

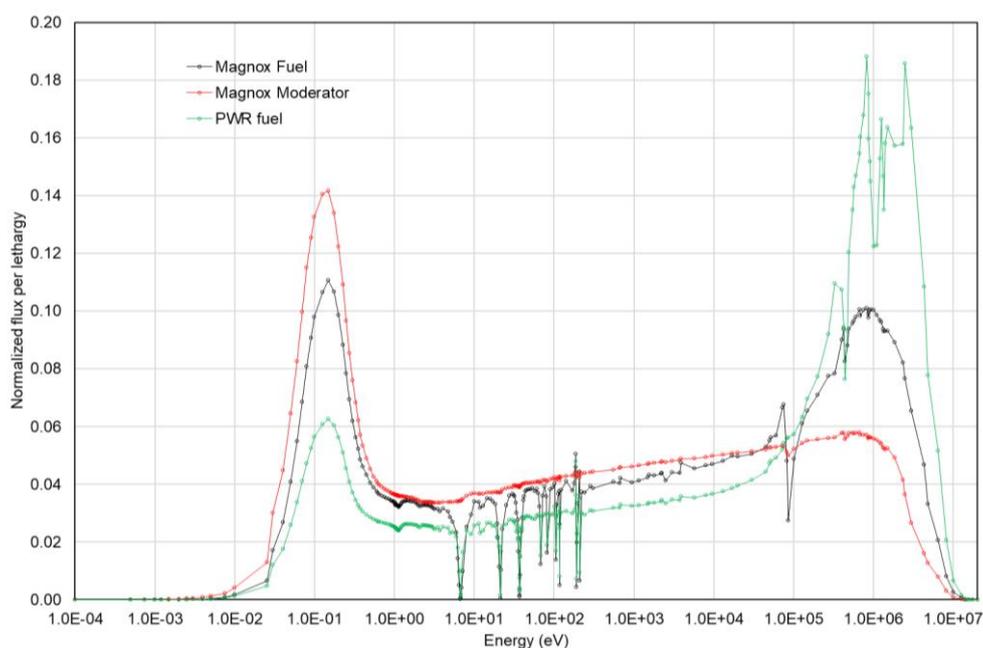


Figure 1. Comparison of neutron spectra between Magnox and PWR.

2.2 MPACT 69-Group Library Generation

2.2.1 AMPX and MPACT MG library generation procedure

The MPACT multigroup (MG) library generation procedure includes seven steps. (a) The AMPX MG library is generated by using temperature-dependent pointwise (PW) weighting functions, which are obtained from the CENTRM [5] PW slowing-down transport calculations. Resonance data are generated by narrow resonance (NR) approximation. (b) Intermediate resonance (IR) parameters are generated, and resonance data are updated with new data, which are obtained by the CENTRM homogeneous slowing-down calculations using LAMBDA and IRFFACTOR-hom [8], as shown in Figure 2. (c) Resonance data are updated with new data calculated by the CENTRM heterogeneous slowing-down calculations for important resonance nuclides using IRFFACTOR-het [8]. (d) Subgroup data are generated for the selected nuclides by using SUBGR [8]. (e) Transport correction factors are generated for ^1H and graphite by performing a fixed-source transport calculation. (f) MG background cross sections are obtained for most nuclides and to collect transient data. (g) The final step is to generate the final MPACT MG library with the data prepared at steps (a) through (f) by using DECLIB.

Figure 2 provides a flow diagram of DECLIB to generate the MPACT MG library. The required data for the steady-state transport calculation are the transport cross section, the fission cross section, the average number of neutrons released from a fission reaction, and the fission spectrum for each nuclide. Since the absorption and fission cross sections are modified through the resonance treatment and are needed for the depletion calculation, those cross sections should be included. The (n,2n) and (n,3n) cross sections are also included for depletion calculations. High order ($P_1 \sim P_3$) scattering matrices are also included.

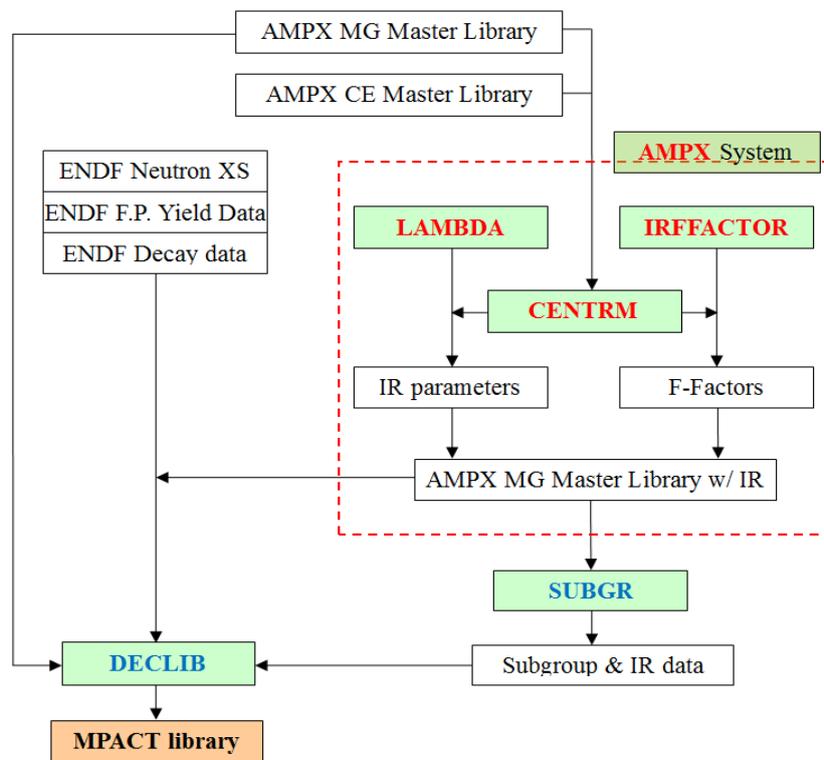


Figure 2. Flow chart to generate the MPACT MG library.

2.2.2 New 69-group structure

The primary option for a scattering source in MPACT is a transport-corrected P_0 calculation to save computing time. To avoid negative flux and convergence issue during 3D whole-core calculation, the MPACT 51-group structure was developed to have evenly distributed lethargy widths for the PWR analysis. In addition, the 51-group structure was developed to be a subset of the SCALE 252-group structure. Simple single-pin benchmark problems were developed for Magnox and the benchmark calculations were performed using the VERA MPACT with the ENDF/B-VII.1 MPACT 51- and 252-group libraries and the SCALE CE-KENO to obtain reference solutions. And then reaction rate analysis was performed to address deficiency of the MPACT 51-group structure and to identify which groups should be refined based on the 252-group structure. The procedure of the detailed reaction rate analysis can be found in reference [9]. Detailed reaction analysis indicated that more thermal energy groups need to be added. Therefore, the 69-group structure was developed by adding 14 thermal and 4 epithermal groups to the 51-group structure to have relatively evenly distributed lethargy widths and to be a subset of the SCALE 252-group structure. Figure 3 provides a comparison of 69-, 51-, and 252-group structures.

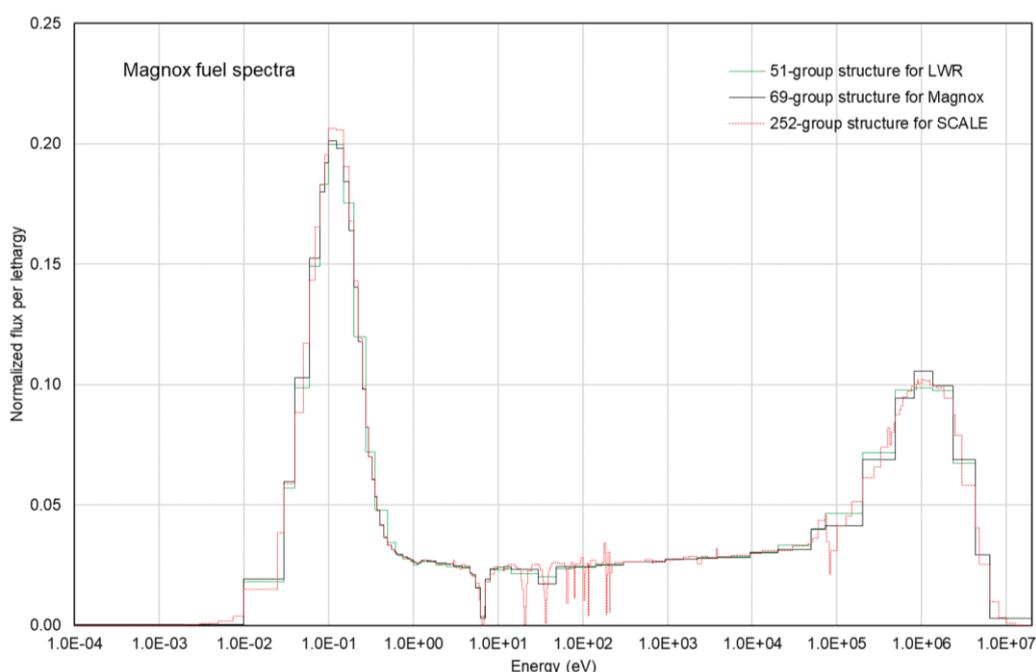


Figure 3. Comparison of energy group structures.

2.2.3 Transport correction factors for graphite

Transport correction factors for graphite based on the NLC method [10] have been generated by using the SCALE procedure, HTransportXS, which is based on SCALE-XSDRN with discrete ordinate (S_N) diamond differencing. The shape of the graphite transport corrections factors is very different from the shape of ^1H in water, and the transport effect of graphite is much greater than that of ^1H in water. Figure 4 shows transport correction factors for graphite and ^1H in water. Transport correction factors were obtained at the ENDF/B-VII.1 temperatures for $S(\alpha,\beta)$ bound nuclide thermal scattering data and then the factors were used in obtaining transport cross sections for graphite.

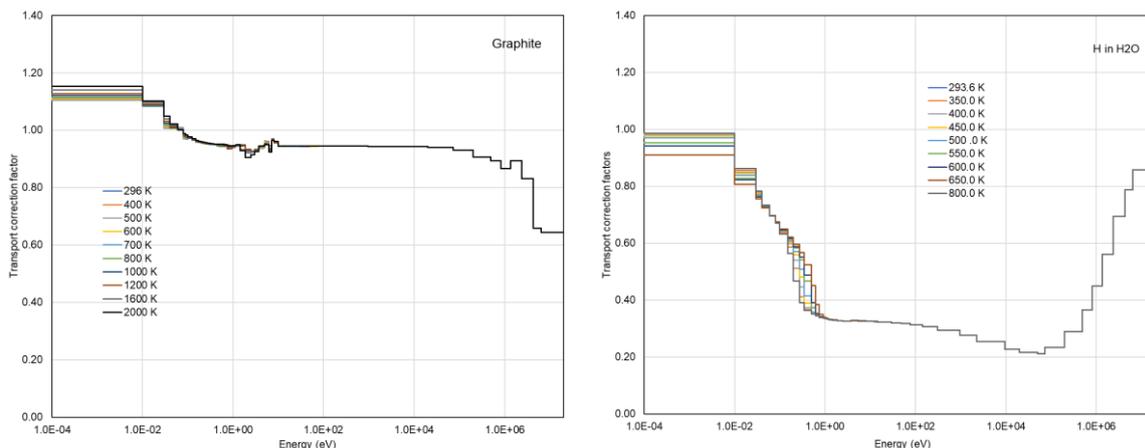


Figure 4. Transport correction factors for graphite and ¹H in H₂O.

2.2.4 SPH Factor Generation

Figure 5 shows a procedure to obtain the SPH factors for ²³⁸U to conserve reaction rates between the CE-KENO reference solutions and the MPACT results for which the CE-KENO models include the same variation cases as the heterogeneous IRFFACTOR cases. The SPH factors can be selectively applied to the specified energy groups, indicating significant reaction rate differences from reaction rate analysis. There is a limitation in conserving reaction rates only by adjusting self-shielded cross sections for thermal groups because Magnox fuel includes a massive thermal peak. Therefore, thermal scattering matrices of the MPACT 69-group library for important nuclides were updated using the SCALE-XSProc-produced P₀ and P₁ thermal scattering matrices.

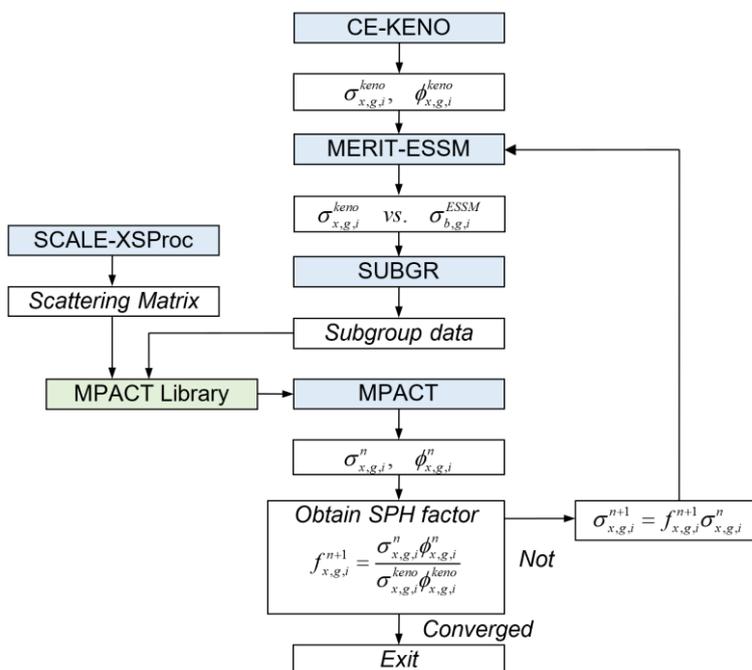


Figure 5. Procedure to generate the SPH factors.

2.2.5 ENDF/B-VII.1 MPACT 69-group library generation

The ENDF/B-VII.1 MPACT 69-group library was developed using the SCALE/AMPX and VERA-XSTools code packages. Only selected resonance nuclides include heterogeneous resonance F-factors; they have been determined to be important resonance nuclides because they can significantly impact the neutronics result. The 14 nuclides listed below were selected to have heterogeneous resonance F-factors based on detailed reaction rate analysis for representative benchmark cases with various burnup and temperatures. The subgroup data for these nuclides were generated using a method to conserve self-shielded cross sections.

- ^{133}Cs , ^{155}Eu , ^{167}Er , ^{232}Th , ^{233}U , ^{235}U , ^{236}U , ^{238}U , ^{238}Pu , ^{239}Pu , ^{240}Pu , ^{241}Pu , ^{242}Pu , and ^{241}Am

The Bondarenko resonance F-factors in the AMPX MG library should be converted into resonance integral tables to be used in subgroup data generation. Next, the subgroup data are generated by using SUBGR. Subgroup data, including weights and levels, were generated for 52 important resonance nuclides as shown in Table I. The following data files are required for DECLIB to generate the MPACT 69-group library:

- ENDF/B-VII.1 AMPX 69-group library
- ENDF/B-VII.1 files: neutron data, decay constants, and fission product yields
- subgroup data and resonance integral table (52 nuclides, groups 10–35 in 69-group structure)
- transport correction factors for graphite
- predetermined background cross sections based on single fuel pin with 10 MWD/kgU burnup (158 nuclides)
- transient data (21 nuclides)

Table I. List of nuclides including subgroup data.

No	Nuclide								
1	^{91}Zr	12	^{123}Sb	23	^{156}Gd	34	^{177}Hf	45	^{236}U
2	^{96}Zr	13	^{124}Sb	24	^{157}Gd	35	^{178}Hf	46	^{238}U
3	^{95}Mo	14	^{131}Xe	25	^{158}Gd	36	^{179}Hf	47	^{238}Pu
4	^{99}Tc	15	^{133}Cs	26	^{160}Dy	37	^{180}Hf	48	^{239}Pu
5	^{103}Rh	16	^{152}Sm	27	^{161}Dy	38	^{182}W	49	^{240}Pu
6	^{108}Pd	17	^{151}Eu	28	^{162}Dy	39	^{183}W	50	^{241}Pu
7	^{107}Ag	18	^{152}Eu	29	^{163}Dy	40	^{184}W	51	^{242}Pu
8	^{109}Ag	19	^{153}Eu	30	^{164}Dy	41	^{186}W	52	^{241}Am
9	^{113}In	20	^{154}Eu	31	^{166}Er	42	^{232}Th		
10	^{115}In	21	^{155}Eu	32	^{167}Er	43	^{233}U		
11	^{121}Sb	22	^{155}Gd	33	^{176}Hf	44	^{235}U		

2.3 Benchmark Calculations

2.3.1 Benchmark problems

A simple benchmark problem was developed using the geometry and composition specifications provided in Table II. This model was used as a reference case in the IRFFACTOR heterogeneous models with various variations to achieve a wide range of background cross sections to complete the resonance F-factor tables.

In addition, the same models with five temperatures (293, 600, 900, 1200, and 2400 K) of the AMPX MG library were used to obtain the ^{238}U SPH factors to conserve reaction rates. The reference solutions were obtained using the SCALE CE-KENO with ENDF/B-VII.1, and the VERA MPACT calculations were performed with the ENDF/B-VII.1 MPACT 51-, 252-, and 69-group libraries. Furthermore, the same benchmark calculations were performed using the SCALE MG procedure based on the CENTRM PW slowing down calculations with the ENDF/B-VII.1 AMPX 252- and 1597-group libraries.

Table II. Specification of geometry and composition.

Zone	Material	Radius (cm)	Atomic number density (/barn-cm)			
Fuel	Natural uranium	1.46	^{235}U	3.48849E-04	^{238}U	4.74655E-02
Clad	Magnox	2.04	^9Be	5.81354e-06	^{24}Mg	3.37805E-02
			^{25}Mg	4.27655E-03	^{26}Mg	4.70848E-03
			^{27}Al	3.10687E-04		
Coolant	CO_2	5.28	C	1.10838E-04	^{16}O	2.21739E-04
Moderator	Graphite	20.32 (pitch)	^{10}B	1.82903E-08	^{11}B	7.36208E-08
			Graphite	8.27968E-02		

2.3.2 Benchmark results

Table III provides a comparison of the benchmark results using various codes and libraries. The MPACT results with the MPACT 69-group library are very consistent with the CE-KENO results for all temperatures and even better than the 252-group MPACT results. The reason that the 252-group MPACT results are poor is that any SPH factors were not applied to ^{238}U to conserve reaction rates. Most of the reactivity differences between CE-KENO and MPACT with the 252-group library come from poor thermal scattering matrices, no consideration of angle-dependent total cross section, and no high-order flux moment weighting for scattering matrices. The SCALE MG results based on the CENTRM PW slowing down calculation with the AMPX 252- and 1597-group libraries were also compared to the CE-KENO and VERA MPACT results. The 69-group MPACT results are comparable to the SCALE 1597-group results. Therefore, it can be noted that the MPACT 69-group library works reasonably well for Magnox reactor analysis.

Table III. Comparison of the multiplication factors.

Temp (K)		CE-KENO K_{inf} [1]	VERA MPACT						SCALE MG			
Fuel	Non-fuel		K_{inf}			$\Delta\rho$ (pcm)			K_{inf}		$\Delta\rho$ (pcm)	
			51-g [2]	252-g [3]	69-g [4]	[1-2]	[1-3]	[1-4]	252-g [5]	1597-g [6]	[1-5]	[1-6]
293	293	1.07201	1.05980	1.06931	1.07170	-1075	-236	-27	1.07070	1.07120	-114	-71
600	600	1.05718	1.04513	1.05372	1.05715	-1090	-311	-3	1.05564	1.05635	-138	-74
900	600	1.05313	1.04093	1.04962	1.05310	-1113	-317	-3	1.05183	1.05249	-117	-58
1200	600	1.05007	1.03767	1.04639	1.05010	-1138	-335	3	1.04885	1.04940	-111	-61
2400	600	1.04105	1.02734	1.03717	1.04073	-1282	-359	-30	1.03983	1.04040	-113	-60

3. CONCLUSIONS

Neutronic characteristics of Magnox reactors are very different from those of PWR due to the graphite moderator. The Magnox neutron spectrum is much softer than the PWR spectrum and the diffusion length

of the Magnox fuel is much longer than that of PWR. Therefore, more energy groups are required for thermal energy ranges. A new 69-group structure was developed by adding more thermal energy groups to the MPACT 51-group structure for PWR. The group structure was devised to be evenly distributed for the transport-corrected P_0 scattering calculations and to be a subset of the SCALE 252-group structure. To improve poor thermal spectra, effective thermal scattering matrices were explicitly obtained from the CENTRM PW slowing down calculation for the typical Magnox fuel pin. Benchmark results in this paper and the companion paper [12] indicate that the ENDF/B-VII.1 MPACT 69-group library have been successfully developed for Magnox reactor analysis using the AMPX/SCALE and VERA-XSTools code packages.

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