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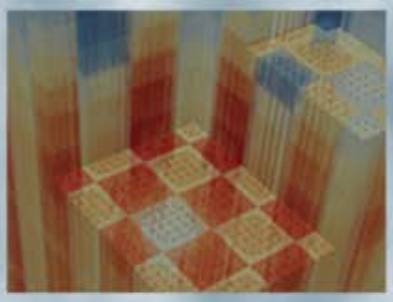
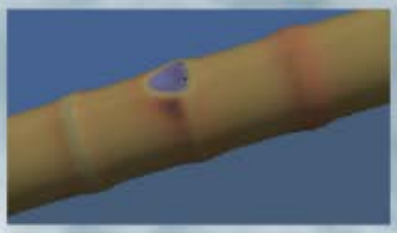
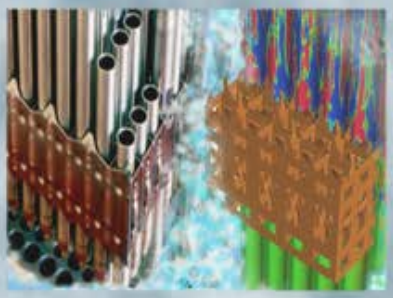
Development of a New 47-Group Library for the CASL Neutronics Simulator







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DEVELOPMENT OF A NEW 47-GROUP LIBRARY FOR THE CASL NEUTRONICS SIMULATORS

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ABSTRACT

The MPACT neutronics module of the Consortium for Advanced Simulation of Light Water Reactors (CASL) core simulator is a 3-D whole core transport code being developed for the CASL toolset, Virtual Environment for Reactor Analysis (VERA). MPACT is under development for neutronics and thermal-hydraulics coupled simulation for pressurized light water reactors. Key characteristics of the MPACT code include (1) a subgroup method for resonance self-shielding and (2) a whole core solver with a 1-D / 2-D synthesis method. Oak Ridge National Laboratory (ORNL) AMPX/SCALE code packages have been significantly improved to support various intermediate resonance self-shielding approximations such as subgroup and embedded self-shielding methods. New 47-group AMPX and MPACT libraries, which are based on ENDF/B-VII.0, have been generated for the CASL neutronics module MPACT. The MPACT group structure comes from the HELIOS library. This new 47-group MPACT library includes all nuclear data required for static and transient core simulations. This study discusses a detailed procedure to generate 47-group AMPX and MPACT libraries and benchmark results for VERA progression problems.

Key Words: CASL, neutronics, MPACT, 47-group, self-shielding

1 INTRODUCTION

A reactor core neutronics simulator called MPACT [1] has been developed to include an advanced pin-resolved transport capability within VERA (Virtual Environment for Reactor Analysis) supported by the Consortium for the Advanced Simulation of Light Water Reactors (CASL). The key characteristics of the MPACT code include the subgroup method [2] and the embedded self-shielding method (ESSM) [3] for resonance treatment. The MPACT code also includes a whole core solver with a 1-D/2-D synthesis method on the frame of the 3-D coarse mesh finite difference (CMFD) method. Axial and radial correction factors are obtained from the 1-D nodal expansion method (NEM) or from the simplified P_N and 2-D method of characteristics (MOC), respectively. In addition, the CASL neutronics simulator MPACT includes various reactor core simulation capabilities such as burnup, as well as transient and thermal-hydraulic feedback calculations. These methods are somewhat similar to those of other forgoing whole neutronics simulators such as DeCART [4] and nTRACER [5]. Thus the MPACT code requires a cross section library to support all the MPACT core simulation capabilities.

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The AMPX code package [6] has been developed at Oak Ridge National Laboratory (ORNL) to generate the multigroup (MG) and continuous energy (CE) AMPX libraries for the SCALE code package [7] by processing the evaluated nuclear data such as ENDF/B and JEFF. The SCALE MG procedure computes problem-dependent MG cross sections through a combination of the conventional Bondarenko calculation and a deterministic pointwise (PW) slowing down calculation of the fine-structure spectra in the resolved resonance and thermal energy ranges. BONAMI is a module of the SCALE system that is used to perform the Bondarenko calculations for resonance self-shielding. CENTRM computes PW neutron spectra in 0-D, 1-D or 2-D systems by solving the Boltzmann transport equation using a combination of PW and MG nuclear data. In SCALE, CENTRM is used mainly to generate self-shielded MG cross sections for subsequent analysis. While the computational accuracy of SCALE would not be significantly influenced by the MG AMPX resonance data, the MPACT self-shielding calculation relies only on the Bondarenko approach with a direct utilization of the MG resonance data. Therefore, the AMPX/SCALE code packages required improvement, and the MG resonance data required update for the Bondarenko approach.

A new program, LAMBDA, has been developed to generate the intermediate resonance (IR) parameters. Another new program, IRFFACTOR, was developed to generate the Bondarenko F-factors for the MG AMPX library. These programs have been incorporated into the AMPX/SCALE code packages. The IR parameters were generated using LAMBDA with homogeneous models, and the Bondarenko F-factors were generated by using IRFFACTOR with either a homogeneous or heterogeneous model. The HELIOS 47-group structure [8] has been very successful in completing the 3-D whole core transport calculations, as demonstrated in DeCART and nTRACER. Thus the 47-group AMPX library, based on ENDF/B-VII.0, has been generated.

The subgroup method for resonance self-shielding calculation in MPACT requires subgroup data that are composed of subgroup levels and weights. The standalone subgroup program, SUBGR, has been developed to generate the subgroup data by a least square fitting which utilizes resonance self-shielded cross sections as a function of background cross section converted from the MG AMPX library. The ENDF/B-VII.0 47-group MPACT library in a unique data format has been generated by using the DECLIB program with the 47-group AMPX library and the subgroup data. The CASL neutronics simulator MPACT computes all static and transient core simulations, which also requires transient data such as delayed neutron fractions and decay constants. Since the current MG AMPX library does not support some of transient data, the data have been generated by using the NJOY code package [9] and then incorporated into the 47-group MPACT library. Reference [10] indicates that a significant improvement on fuel temperature coefficient can be achieved through a consideration of epithermal upscattering. An additional set of subgroup data with a consideration of the epithermal upscattering effect has been generated for ^{238}U by Monte Carlo calculations, coupled with ESSM [11] and included in the 47-group MPACT library. In order to accommodate high order scattering accuracy with a transport corrected P_0 (TCP_0) calculation, transport cross sections have been generated for light nuclides by using various transport correction methods [11, 12].

This paper describes a detailed procedure to generate the 47-group AMPX and MPACT libraries, and it includes the MPACT benchmark results for the VERA progression problems [13] for which the reference solutions were obtained by the KENO CE calculations.

2 LIBRARY PROCESSING PROCEDURE

2.1 The Conventional AMPX Procedure

AMPX-6 [6] is a modular system of FORTRAN computer programs to generate the MG and CE cross section libraries for modern deterministic and Monte Carlo transport codes by processing the ENDF/B libraries. Since the CASL neutronics simulator MPACT is a deterministic transport code, only the MG AMPX library generation procedure is discussed. Figure 1 provides the AMPX procedure to generate the MG AMPX library where the left side of flow chart is for the conventional procedure and the right side for new procedure to improve the Bondarenko resonance data.

The MG AMPX library includes various neutron reactions of the Bondarenko F-factors as a function of background cross section for resolved and unresolved resonance groups. The resolved resonance F-factors have been generated by the narrow resonance (NR) approximation and the unresolved ones by the J-function method [14] based on the NR approximation. And MG 1-D and 2-D data have been obtained by using a weighting function which consists of Maxwellian spectrum at thermal, 1/E at epithermal and fission spectrum at fast energy ranges. It should be noted that the 2-D scattering data are temperature independent in the MG AMPX library. In the standard SCALE procedure, self-shielded MG 1-D and 2-D data for resolved resonance and thermal energy groups are determined by performing the CENTRM slowing down transport calculation with Equation (1), and thus the resolved resonance data in the MG AMPX library are insignificant.

$$\hat{\Omega}\cdot\nabla\psi+\Sigma_t(\vec{r},u)\psi(\vec{r},u,\hat{\Omega})=\int_{u-\ln(1/\alpha)}^{u}\frac{\Sigma_s(u')\phi(u')}{(1-\alpha)}e^{u'-u}du', \qquad (1)$$

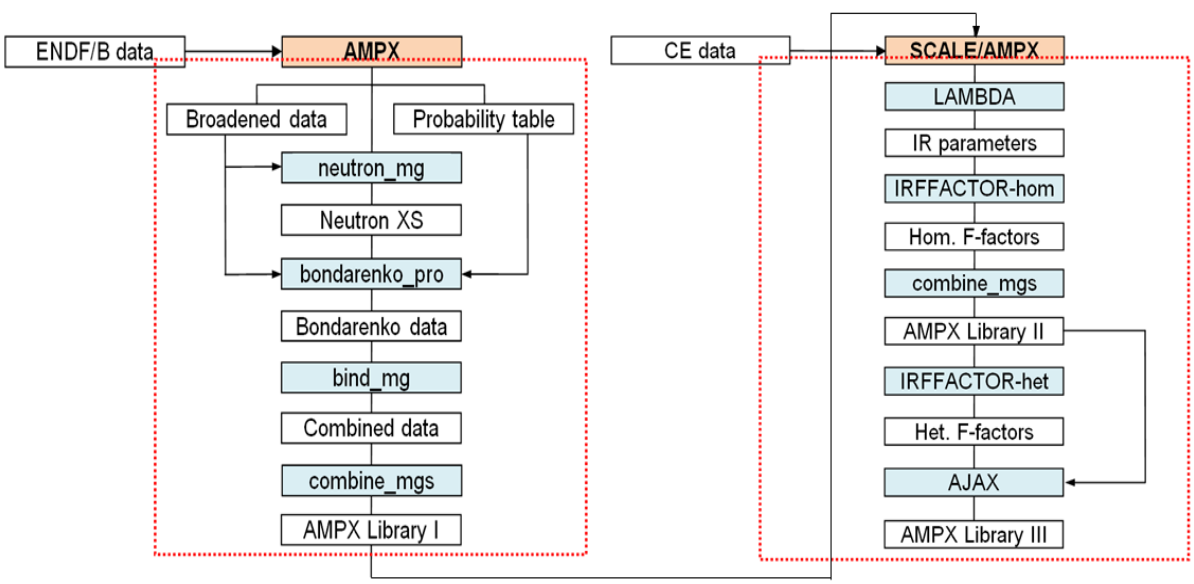


Figure 1. Flow chart of the AMPX procedure

where u denotes lethargy, and ϕ and ψ scalar and angular fluxes, respectively. In Equation 1 Σ_t and Σ_s are total and scattering cross sections, respectively, and α is defined as $(A\text{-}1)^2/(A+1)^2$ where A is atomic mass.

2.2 New AMPX Procedure for the Bondarenko Approach

2.2.1 IR parameter

The IR parameter [15] can be defined as a probability passing through resonance without any reaction which correlates the NR and wide resonance (WR) approximations. Since the atomic mass of hydrogen (^{1}H) is very close to unity, lethargy gain of any neutron colliding with hydrogen is very large, and the neutron can scatter beyond a resonance without any collision. This is essentially the same as the narrow resonance approximation. Therefore, for hydrogen, the intermediate resonance parameter is defined as unity. For other nuclides, the IR parameter is obtained by comparing results of various ^{238}U/^{1}H mixtures where the hydrogen is partly replaced by the other isotopes [16]. This is often referred to as a hydrogen-equivalence parameter.

At first a self-shielded cross section table, $\sigma_{g,a}^{238}$ vs. $\sigma_{g,b}^{238}$, must be prepared by performing slowing down calculations with various hydrogen atomic number densities (N^1) at the fixed ^{238}U atomic number density (N^{238}). The background cross sections can be obtained using the following equation assuming the ^{1}H (λ_g^1) and ^{238}U (λ_g^{238}) IR parameters to be unity.

$$\sigma_{g,b}^{238} = \frac{N^{238}\lambda_g^{238}\sigma_p^{238} + N^1\lambda_g^1\sigma_p^1}{N^{238}} = \frac{\sum_{i=all} N^i\lambda_g^i\sigma_p^i}{N^R}. \tag{2}$$

Then the slowing down calculation is performed for a mixture of ^{238}U, ^{1}H and a target nuclide x. A new $\sigma_{g,a}^{238}$ is calculated, and the corresponding $\sigma_{g,b}^{238}$ is read from the prepared $\sigma_{g,a}^{238}$ table. The IR parameter (λ_g^x) for a nuclide x can be obtained by using Equation (3)

$$\lambda_g^x = \frac{\sigma_{g,b}^{238}N^{238} - N^{238}\lambda_g^{238}\sigma_p^{238} - N^1\lambda_g^1\sigma_p^1}{N^x\sigma_p^x}, \tag{3}$$

where σ_p^x is the potential cross section. The IR parameter of ^{238}U should be determined first, and then the IR parameters of other nuclides should be evaluated. The LAMBDA program in Figure 1 computes all of the IR parameters for all nuclides by using this procedure.

2.2.2 Homogeneous F-factors

The Bondarenko F-factor tables are to be generated by performing homogeneous slowing down calculations with a mixture of ^{1}H and target nuclide. This process is identical to that used for preparing a self-shielded cross section table for the IR parameter as described in Section 2.2.1. The Bondarenko F-factor tables must be determined to cover all background cross sections, from zero to infinity. Figure 2 illustrates the procedure to generate the F-factors by

using IRFFACTOR, which executes CENTRM and performs ESSM. These homogenous F-factors are typically generated for nuclides with atomic mass numbers larger than 40. New Bondarenko F-factors are to be incorporated into the MG AMPX library.

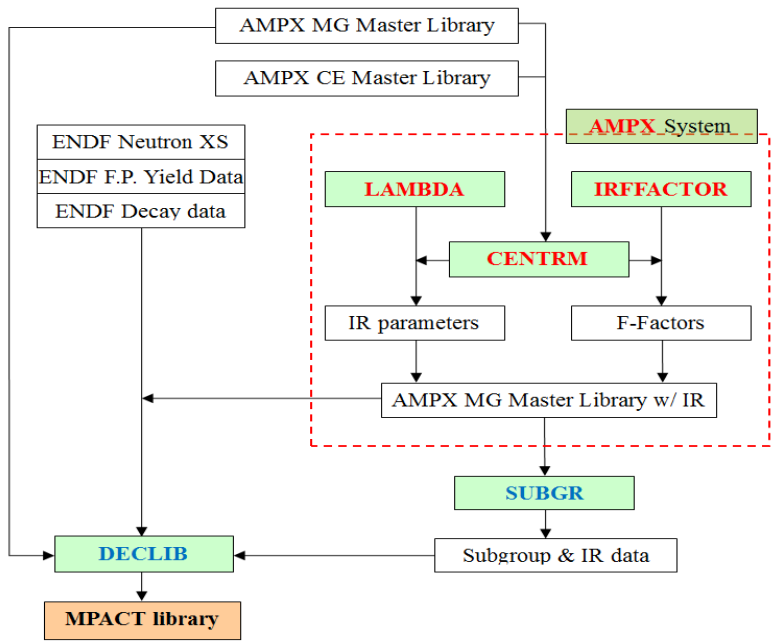


Figure 2. Flow chart of the MPACT library generation procedure

Table I. Example of variations

Case		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Volume	Fuel	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	Clad	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	Mod	1.0	1.0	1.0	1.0	1.0	2.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0
Fuel	^{235}U	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.25	0.125	0.0625	0.03125	0.01	0.01	0.01	0.01
	^{238}U	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.25	0.125	0.0625	0.03125	0.01	0.001	1.0E-6	1.0E-7
	^{16}O	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.25	0.125	0.0625	0.03125	0.01	0.01	0.01	0.01
H_2O	^{1}H	2.5E-3	0.2	0.5	0.75	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	^{16}O	2.5E-3	0.2	0.5	0.75	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

2.2.3 Heterogeneous F-factors

The Bondarenko F-factor tables are also to be generated by using heterogeneous slowing down models, which ensures more precise results compared to those obtained using homogeneous models. As shown in Figure 2, the IRFFACTOR module is responsible for this calculation. The PW slowing down calculations using Equation 1 are performed by using CENTRM for the heterogeneous models, and then the MG self-shielded absorption ($\sigma_{g,a}$), fission ($\sigma_{g,f}$) and scattering ($\sigma_{g,s}$) cross sections are edited. The final step is to estimate the corresponding background cross section by solving the following MG fixed source transport using Equation (4)

and converting the scalar flux (ϕ_g) into a background cross section using Equation (5) based on equivalence theory

$$\hat{\Omega} \cdot \nabla \psi_g + \sum_i (\Sigma_{i,g,a} + \lambda_{i,g} \Sigma_{i,p}) \psi_{g,k}(\hat{\Omega}) = \sum_i \lambda_{i,g} \Sigma_{i,p} \ , \tag{4}$$

$$\sigma_{b,g}^k = \frac{\Sigma_{b,g}}{N_k} = \frac{\Sigma_{a,g} \phi_g}{1 - \phi_g} \ . \tag{5}$$

where k denotes resonant nuclide. Various background cross sections can be achieved by changing geometrical and compositional configurations as shown in Table I.

2.2.4 Monte Carlo based heterogeneous F-factors

No deterministic slowing down program is available to consider epithermal upscattering. Therefore the Bondarenko f-factor tables must be generated by performing the continuous energy Monte Carlo calculations and evaluating the corresponding background cross sections [11]. The F-factor tables can be generated by using either homogeneous or heterogeneous models. The key feature of this procedure is to perform the Monte Carlo calculations to obtain MG self-shielded cross sections instead of solving deterministic PW slowing down calculations. In this study, the KENO CE calculations were performed to edit effective microscopic cross sections rather than the CENTRM slowing down calculations. The corresponding background cross sections can be obtained by the same method described in Section 2.2.2. The Bondarenko F-factors have been obtained by performing the KENO CE calculations without and with the Doppler Broadening Rejection Correction (DBRC) option to consider the resonance upscattering effect.

2.3 Subgroup Data Generation

The subgroup method requires the subgroup data, which can be transformed from the Bondarenko F-factor tables. The essential aspect of the subgroup method is that the effective resonance cross sections are approximated by quadratures in which the resonances are divided into the subgroup levels, and the corresponding subgroup weights are assigned as probabilities. Fixed source transport calculations are performed at each subgroup level, corresponding background cross sections are determined, and then self-shielded cross sections are estimated with a consideration of resonance interference effect between nuclides. As shown in Figure 2, the SUBGR code computes the subgroup data through a nonlinear least square fitting by using the IR parameters and F-factor tables in the MG AMPX library. The IR parameters and F-factor tables are computed using the IRFFACTOR and LAMBDA modules. Subgroup data are composed of the subgroup levels for the absorption, the ν*fission cross sections, and the corresponding temperature-dependent subgroup weights. The subgroup data can be generated by conserving either self-shielded resonance integrals [8] or cross sections [17]. Capabilities for these are included in SUBGR.

2.4 Transport Corrected Cross Sections

The MOC calculation with high order ($\geq P_2$) scattering source requires 2 times longer computing time than the P_0 MOC calculation. Most of transport lattice codes typically perform transport corrected P_0 scattering calculations in which diagonal terms of P_0 scattering matrix are subtracted by total P_1 scattering cross sections or adjusted by other transport correction methods. The P_1 corrected P_0 scattering matrix for ^{1}H may include negative value in the diagonal components. This would cause negative flux, resulting in convergence error. This is still an open problem. The DECLIB code has been developed to consider various transport correction methods, such as typical out-scattering approximation, the nTRACER in-scattering approximation [18] and the neutron leakage conservation (NLC) method [12]. While transport cross sections and transport corrected P_0 scattering matrices with out- and in-scattering approximations can be easily generated, the NLC ones require transport correction factors to be generated independently. A 1-D MOC program with high order scattering has been developed, and the transport correction factors have been evaluated using the method described in Reference [12]. Figure 3 provides the 47-group transport correction factors for ^{1}H with various temperatures.

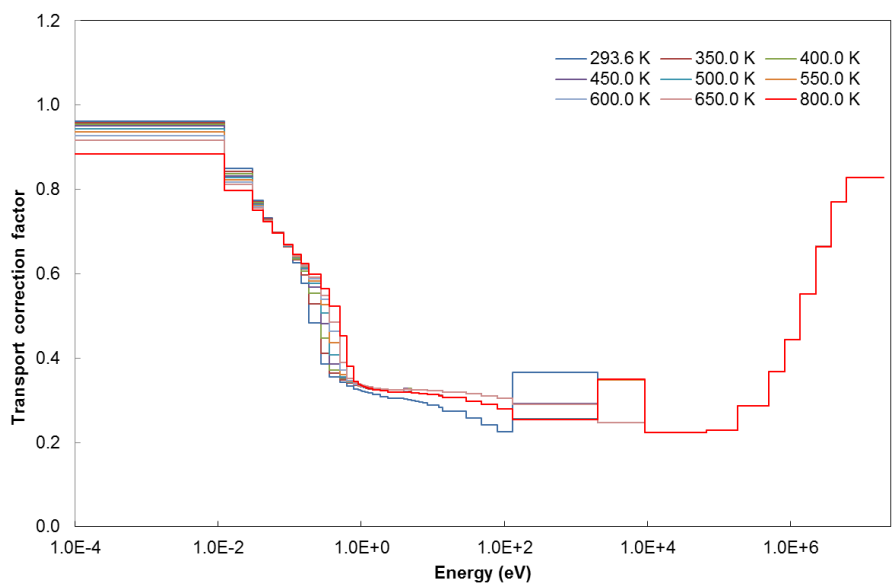


Figure 3. Transport correction factors for ^{1}H

3 LIBRARY GENERATION AND BENCHMARK CALCULATION

3.1 Library Generation

The 47-group AMPX library, which has been generated with the ENDF/B-VII.0 nuclear data, includes 448 nuclides and 5 molecules. Although ENDF/B-VII.0 includes 423 nuclides, some are duplicated in the 47-group AMPX library due to various thermal scattering data for molecules and special purpose in the SCALE code system. A new PW weighting function has

been obtained from the pointwise CENTRM slowing down calculation for a typical pressurized water reactor (PWR) fuel pin configuration and utilized in obtaining 1-D and 2-D MG cross sections instead of using the conventional weighting function with Maxwellian spectrum, 1/E, and fission spectrum. While the Bondarenko F-factors for nuclides with atomic mass numbers (Z) less than 40 have been generated by using the NR approximation, those for $Z \geq 40$ (^{40}Zr) nuclides include the homogeneous F-factors. Only selected nuclides include heterogeneous F-factors, which are very important resonance nuclides that significantly impact the neutronics result. The following 14 nuclides have been selected to have the heterogeneous F-factors.

^{107}Ag, ^{109}Ag, ^{113}Cd, ^{113}In, ^{115}In, ^{154}Gd, ^{155}Gd, ^{156}Gd, ^{157}Gd, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu

The 47-group MPACT library includes 295 nuclides, of which only 49 include resonance integral tables and subgroup data. The resonance energy groups are 9 to 26 out of 47, ranging from 1.4574 eV to 9.1188 eV. Most nuclides include transport cross sections based on out-scattering approximation. Transport cross sections with the NLC transport correction method have been generated only for ^{1}H, and those with the nTRACER in-scattering approximation have been generated for ^{11}B, ^{12}C and ^{16}O.

Since ^{238}U resonance self-shielded cross sections are the most important and dominant in simulating PWR, they have been generated by using the KENO CE + ESSM calculations as described in Sections 2.2.3 and 2.2.4 and converted into subgroup data. In addition, one more set of resonance self-shielded cross section tables and subgroup data has been generated using the same KENO CE + ESSM procedure with a consideration of epithermal up-scattering.

The AMPX code package does not support generating part of the transient data such as decay constants (λ_i) and delayed neutron fractions (β_i) of precursor groups. The ENDF/B-VII.0 library includes delayed neutron data for 21 heavy nuclides by which the transient data have been generated by the NJOY code package [9] and included in the 47-group MPACT library.

3.2 Benchmark Calculations and Results

Benchmark calculations have been performed for the VERA progression problems [13] to determine whether the new 47-group MPACT library works reasonably. Table II provides comparisons of k_{eff} and normalized pin power distributions between the KENO-CE and MPACT results for the VERA progression problems 1 (single fuel pin) and 2 (fuel assembly). The default ray options for the MPACT calculations were 2 polar and 16 azimuthal angles for each quadrant and 0.05 cm ray spacing, but a much finer ray option was applied to the integral fuel burnable absorber (IFBA)-bearing cases. Two options for scattering source have been tried using the NLC transport corrected P_0 and pure P_2. The MPACT NLC P_0 and P_2 results for k_{eff} and pin power distributions are very consistent with the KENO-CE results except for the NLC P_0 results for 2g and 2h, which are the control rod inserted cases. The maximum difference of k_{eff} between the MPACT P_2 and KENO CE is 140 per cent mille (pcm), and the root mean square (RMS) and maximum pin power differences are 0.26 % and 0.82 %, respectively. It has been observed that various transport corrected P_0 calculations would not be able to properly simulate the highly anisotropic effect of the control rod inserted cases.

Since VERA progression problems 1 and 2 include single ^{235}U enrichment, additional

benchmark calculations have been performed for problems 1b and 2b with various ^{235}U enrichments ranging from 2.1 w/o to 4.6 w/o. Table III compares calculated k_{eff} values between the MPACT and KENO-CE results. It is noted that the new 47-group MPACT library does not include any ^{235}U enrichment bias at all and thus can be applied to any ^{235}U enrichment less than 4.95 w/o.

Table II. Comparison of k_{eff} and pin powers for the VERA progression problems 1 and 2

Case	Description	KENO	MPACT NLC TCP_0			MPACT P_2		
			Δk (pcm)	RMS	Max.	Δk (pcm)	RMS	Max.
1a	Single pin, T_F=565 K	1.18704	-78	-	-	-54	-	-
1b	Single pin, T_F=600 K	1.18215	-19	-	-	-6	-	-
1c	Single pin, T_F=900 K	1.17172	-9	-	-	1	-	-
1d	Single pin, T_F=1200 K	1.16260	-16	-	-	-10	-	-
1e	Single pin, T_F=600 K, IFBA	0.77169	-143	-	-	-108	-	-
2a	FA, T_F=565 K	1.18218	-104	0.12%	0.22%	-71	0.11%	0.20%
2b	FA, T_F=600 K	1.18336	-38	0.09%	0.20%	-24	0.08%	0.18%
2c	FA, T_F=900 K	1.17375	-12	0.09%	0.18%	-2	0.08%	0.15%
2d	FA, T_F=1200 K	1.16559	-34	0.08%	0.17%	-28	0.07%	0.13%
2e	FA, T_F=600 K, 12 Pyrex	1.06963	8	0.06%	0.15%	-36	0.10%	0.21%
2f	FA, T_F=600 K, 24 Pyrex	0.97602	66	0.11%	0.24%	-11	0.11%	0.29%
2g	FA, T_F=600 K, AIC-CR	0.84770	346	0.24%	0.57%	102	0.20%	0.37%
2h	FA, T_F=600 K, B_4C-CR	0.78822	397	0.26%	0.65%	43	0.21%	0.40%
2i	FA, T_F=600 K, Instrument Thimble	1.17992	-78	0.09%	0.21%	-47	0.08%	0.18%
2j	FA, T_F=600 K, IT+24 Pyrex	0.97519	74	0.10%	0.22%	-2	0.11%	0.19%
2k	FA, T_F=600 K, Zoned + 24 Pyrex	1.02006	68	0.11%	0.26%	-2	0.12%	0.21%
2l	FA, T_F=600 K, 80 IFBA	1.01892	-124	0.14%	0.29%	-108	0.08%	0.21%
2m	FA, T_F=600 K, 128 IFBA	0.93880	-148	0.15%	0.31%	-124	0.08%	0.17%
2n	FA, T_F=600 K, 104 IFBA+20 WABA	0.86962	-90	0.14%	0.29%	-140	0.10%	0.24%
2o	FA, T_F=600 K, 12 Gadolinia	1.04773	42	0.14%	0.30%	-45	0.14%	0.33%
2p	FA, T_F=600 K, 24 Gadolinia	0.92741	29	0.19%	0.48%	-131	0.19%	0.36%
2q	FA, T_F=600 K, Zircaloy SG	1.17194	-54	0.24%	0.72%	-30	0.26%	0.82%

Table III. Comparison of multiplication factors for various ^{235}U enrichments

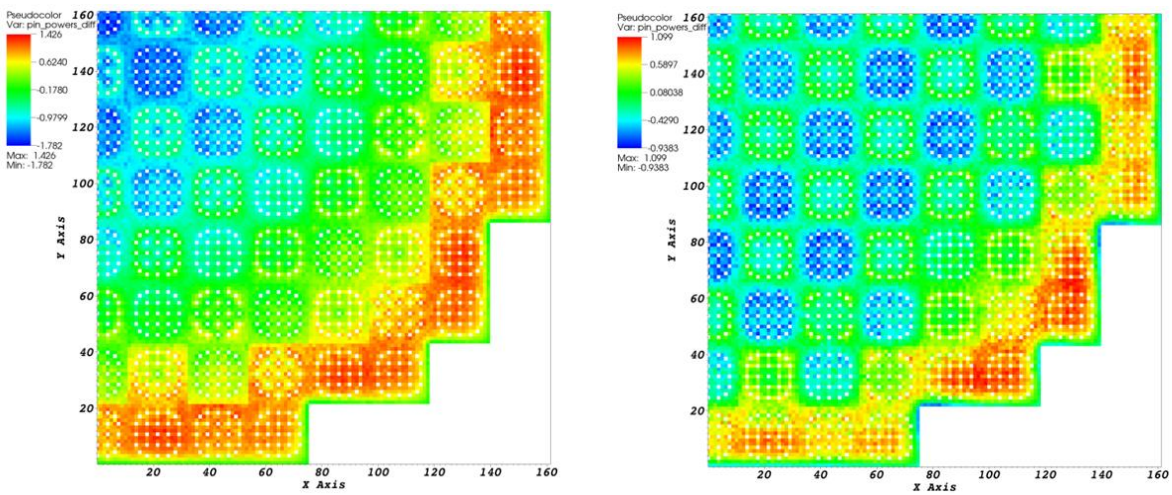
^{235}U w/o	Pin (1b)			Assembly (2b)		
	MPACT	KENO-CE	Δk (pcm)	MPACT	KENO-CE	Δk (pcm)
2.1	1.07028	1.07034	-6	1.06135	1.06138	-2
2.6	1.13548	1.13569	-21	1.13061	1.13060	1
3.1	1.18226	1.18217	9	1.18349	1.18360	-11
3.6	1.22114	1.22118	-4	1.22523	1.22527	-4
4.1	1.25257	1.25271	-14	1.25904	1.25915	-11
4.6	1.27857	1.27879	-22	1.28703	1.28726	-23

*S.D.: 0.00018 for pin / 0.00009 for assembly

In addition, benchmark calculations have been performed for the VERA progression problems 1 through 5, which are hot zero power 2-D whole core problems with and without control rod insertions. Temperatures for all material zones have been assumed to be 565 K. The default ray option—2 polar and 16 azimuthal angles for each quadrant and 0.05 cm ray spacing—has been used, and the NLC P_0 and P_2 calculations have been performed. The MPACT k_{eff} and pin power distributions have been compared with the KENO-CE distributions, as shown in Table IV. The maximum k_{eff} difference between the KENO-CE and MPACT results is 45 pcm. The MPACT NLC TCP_0 calculation provides better results in pin power distribution compared to the P_2 calculation, which might not seem to be reasonable. As shown in Figures 4 (a) and (b), there are slight radial power tilts which need to be addressed.

Table IV. Comparison of k_{eff} for 2-D core (KENO vs. MPACT P_2 and NLC TCP_0)

Case	Description	k_{eff}	MPACT P_2			MPACT NLC TCP_0		
			Δk (pcm)	RMS (%)	Max. (%)	Δk (pcm)	RMS (%)	Max. (%)
5a	Uncontrolled	1.00409	-45	0.76	1.79	-43	0.49	1.15
5b	AIC Controlled	0.99150	-34	0.94	1.99	-32	0.51	1.29
5c	B4C Controlled	0.99023	-35	0.97	2.28	-33	0.52	1.33



(a) KENO-CE vs. MPACT P_2 (b) KENO-CE vs. MPACT NLC TCP_0

Figure 4. Comparison of pin power distribution

Benchmark calculations have been performed for the PWR single fuel pin with various fuel temperatures to obtain fuel temperature coefficients by using MPACT and KENO-CE. While the reference KENO-CE calculations have been performed with and without the DBRC option for ^{238}U, the MPACT calculations have been performed with two different sets of ^{238}U subgroup data, including and excluding epithermal upscattering. Figure 5 provides a comparison of fuel temperature coefficients with and without epithermal upscattering. There are approximately 5 to 13 % relative differences between the fuel temperature coefficients with and without considering

epithermal upscattering. The MPACT results are very consistent with the reference KENO-CE results.

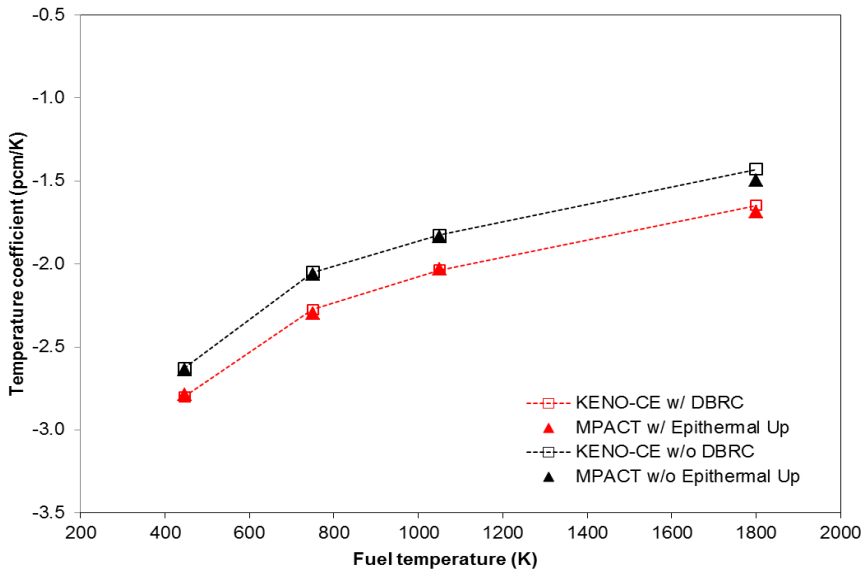


Figure 5. Comparison of fuel temperature coefficients

4 CONCLUSIONS

Resonance self-shielding calculations in the CASL neutronics simulator MPACT are based on the Bondarenko approaches such as the subgroup method and ESSM. In order to support the MPACT resonance self-shielding methodologies, the ORNL AMPX/SCALE code packages have been significantly improved to generate (1) the IR parameters, (2) the Bondarenko F-factors by using homogeneous and heterogeneous models, and (3) the subgroup data. New modules have been developed, including LAMBDA for the IR parameter, IRFFACTOR for the F-factors, and SUBGR for the subgroup data.

The 47-group AMPX and MPACT libraries based on ENDF/B-VII.0 have been successfully generated for the CASL neutronics simulator MPACT by using the new AMPX/SCALE code packages. All nuclides in the AMPX 47-group library include the IR parameters. Nuclides with $Z \geq 40$ include homogeneous F-factors, and heterogeneous F-factors have been generated for 14 important resonant nuclides. The 47-group MPACT library has various discriminating data, such as subgroup data, resonance data considering epithermal upscattering, transient data, and transport cross sections with various approximation methods. It is noted that the computational benchmark results show the 47-group MPACT library working reasonably for various PWR fuel configurations. Further improvements are planned to the 47-group MPACT library, which is based on ENDF/B-VII.0, that should lead to better accuracy and application capability for PWR neutronics analysis.

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6 REFERENCES

1. *MPACT: User's Manual Version 1.0.0*, November 8, 2013.
2. A. Khairallah and J. Recolin, "Calcul de l'autoprotection résonnante dans les cellules complexes par la méthode des sous-groupes," *Proc. Seminar IAEA-SM-154 on Numerical Reactor Calculation*s, pp. 305–317, I.A.E.A., Vienna (1972).
3. Mark L. Williams, Kang-Seog Kim, "The Embedded Self-Shielding Method," *PHYSOR 2012*, Knoxville, Tennessee, USA, April 15–20, 2012 (2012).
4. J. Y. Cho, H. G. Joo, Kang-Seog Kim, S. Q. Zee, "Cell Based CMFD Formulation for Acceleration of Whole-core Method of Characteristics Calculation," *Journal of the Korean Nuclear Society*, **34**, No.3, 250–258 (2002).
5. Y. S. Jung, C. B. Shim, C. H. Lim, H. G. Joo, "Practical numerical reactor employing direct whole core neutron transport and subchannel thermal/hydraulic solvers," *Ann. Nucl. Energ.*, **62**, 357–374 (2013).
6. D. Wiarda, S. Goluoglu, M.E. Dunn, N.M. Green and L. M. Petrie, "AMPX-6: A Modular Code System for Processing ENDF/B Evaluations," in preparation (2014).
7. "SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation," ORNL-TM/2005/39, Version 6, Vols. I–III, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2009). (Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-750.)
8. R. J. J. Stamm'ler et al., "The HELIOS Methods," Studsvik Scandpower (1998).
9. R. E. MacFarlane, D. W. Muir, "The NJOY Nuclear Data Processing System Version 91," LA-12740-M Manual (1994).
10. D. J. Lee, K. Smith, and J. Rhodes, "The Impact of ^{238}U Resonance Elastic Scattering Approximations on Thermal Reactor Doppler Reactivity," *Ann. Nucl. Energy*, 36, 274–280 (2009).
11. Kang-Seog Kim et al., "Monte Carlo Resonance Treatment for the Deterministic Transport Lattice Codes," *Journal of the Korean Nuclear Society*, **35**, No.6, 581–595 (2003).
12. Bryan R. Herman, Benoit Forget, Kord Smith, "Improved Diffusion Coefficients Generated From Monte Carlo Codes," M&C 2013, Sun Valley, Idaho, May 5–9, 2013.
13. Andrew T. Godfrey, "VERA Core Physics Benchmark Progression Problem Specifications," CASL-U-2012-0131-004 R4, http://www.casl.gov/publications.shtml (2014).
14. C. H. Lee and W. S. Yang, "MC^2-3: Multigroup Cross Section Generation Code for Fast Reactor Analysis," ANL-NE-11-41, Argonne National Laboratory (2011).

15. R. Goldstein and E. R. Cohen, "Theory of Resonance Absorption of Neutrons," *Nucl. Sci. Eng*., **13**, 132 (1962).
16. F. Leszczynski, "Neutron Resonance Treatment with Details in Space and Energy for Pin Cells and Rod Clusters," *Ann. Nucl. Energy*, 14, 589–601 (1987).
17. H. G. Joo and et al., "Subgroup Weight Generation Based on Shielded Pin-Cell Cross Section Conservation," *Ann. Nucl. Energ.*, 36, 859 (2009).
18. Min Ryu et al., "Incorporation of Anisotropic Scattering in nTRACER," *Transaction of the Korean Nuclear Society Autumn Meeting*, Pyeongchang, Korea, October 30–31, 2014.