# MULTIGROUP DATA PROCESSING FOR THE EMBEDDED SELF-SHIELDING METHOD IN SCALE<sup>\*</sup>

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### ABSTRACT

The embedded self-shielding method (ESSM) was previously developed to provide an integrated approach for lattice calculations. ESSM consists of three interrelated components: (1) processing multigroup cross sections, (2) computing resonance-shielded multigroup cross sections, and (3) performing neutron transport calculations in lattice physics calculations. The self-shielding computation in ESSM is embedded within the transport solution, which provides information for treating heterogeneous self-shielding effects. The resulting shielded cross sections provide data for the transport calculation. This approach integrates the self-shielding and transport components of the lattice physics calculations. Earlier publications have described this aspect of ESSM; however, another equally important aspect of ESSM is that the processing of the multigroup cross section library is integrated with the self-shielding procedure in a consistent manner. This paper describes the procedures that have been developed to generate multigroup libraries for ESSM calculations of light water reactor lattices with the SCALE code system. Results of sample lattice physics calculations are presented to illustrate the impact of ESSM processing procedures.

Key Words: self-shielding, multigroup processing, AMPX, SCALE-Polaris

#### **1. INTRODUCTION**

This paper describes a method called the *embedded self-shielding method* (ESSM) [1] that has been developed for lattice physics calculations with the SCALE computation system [2]. ESSM is fundamentally a variation of the extensively used Bondarenko method [3]. However, ESSM provides tighter integration between multigroup (MG) library processing, neutron transport, and self-shielding calculations. The general Bondarenko method uses precomputed MG shielding factors (i.e., *f-factors*) that are tabulated as a function of background cross section ( $\sigma_0$ ) and temperature within a problem-independent MG library. The background cross sections and associated f-factors are called *Bondarenko data*. Pregeneration of the Bondarenko data requires that the flux spectrum used to process the f-factors is parameterized in terms of the parameter  $\sigma_0$ , which indicates the degree of self-shielding. The shielded cross section is the product of the shielding factor  $f(\sigma_0)$  and

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the unshielded (infinitely dilute) cross section,  $\sigma_{\infty}$ . To obtain a problem-dependent self-shielded cross section for a given group and a particular assembly lattice configuration, the appropriate background cross section of the lattice is computed, and the corresponding shielding factor is interpolated from the tabulated values on the library.

The primary difference between ESSM and the standard Bondarenko method is in how the parameterized flux spectrum is obtained and how the background cross section is defined. In conventional Bondarenko methods, f-factors are computed from an analytical expression based on the intermediate resonance (IR) approximation for the flux spectrum in an infinite homogenous medium. These values are applied to heterogeneous lattice systems by using equivalence theory to obtain the equivalent background cross section [4]. In contrast, the libraryf-factors for ESSM are evaluated using continuous-energy (CE) flux spectra from deterministic calculations of the neutron transport equation. Either homogeneous media or two-dimensional (2D) heterogeneous cell models can be specified for the CE transport solution, but the most important resonance absorber nuclides-such as uranium and plutonium isotopics-are normally treated using a heterogeneous unit cell model. For a given heterogeneous model, the corresponding library  $\sigma 0$  for each group is obtained by solving one-group fixed-source transport calculations for the unit cell. When the library Bondarenko data are applied in lattice physics simulation, a similar one-group, fixed-source transport calculation is performed for the 2D fuel assembly model to obtain  $\sigma_0$  values for each cell. From these values, self-shielded MG cross sections are obtained by interpolation of the library  $f(\sigma_0)$  factors. Because the ESSM library is processed using heterogeneous cells tailored for a particular class of problems (e.g. LWRs), the accuracy is greatly improved over traditional Bondarenko approaches that rely on homogeneous-heterogeneous equivalence theory. Although the processed f-factors may not be applicable to systems dramatically different from the reference class of heterogeneous lattices, an ESSM library could be developed with appropriate heterogeneous cells that would enable ESSM to accurately model such a system (such as thorium-fueled FHRs).

An important feature of ESSM as implemented in SCALE is that the MG library processing and the self-shielding techniques are integrated in a consistent manner. Consistency between the library Bondarenko processing and the lattice physics self-shielding is an essential component of the overall ESSM methodology, and it is necessary to obtain accurate results. A recent paper by Gibsen, Smith, and Forget [5] presented results obtained with ESSM using cross section data processed with the traditional Bondarenko approach, and showed the computed eigenvalues did not agree well with CE Monte Carlo calculation for several simplistic models. However, results for realistic LWR lattices can be significantly improved by using a processed MG library with f-factors based on heterogeneous cell calculations, consistent with the ESSM definition for the background cross sections. The procedures presented herein are used by Oak Ridge National Laboratory (ORNL) to process MG libraries for ESSM self-shielding calculations in SCALE 6.2, which will be distributed in 2016. This paper demonstrates that accurate results for LWR lattices are obtained with the fully consistent ESSM methodology when these processing procedures are used to generate the MG library.

## 2. PROCESSING OF ESSM SELF-SHIELDING DATA

ESSM provides a methodology that unifies MG data processing, self-shielding, and lattice physics analysis in a consistent manner for light water reactor (LWR) assembly calculations. That is, the flux spectra used to process the MG library are consistent with the self-shielding and MG transport

methods in the heterogeneous lattice calculations. ESSM has been implemented in a SCALE LWR lattice physics module and shown to give good results for an extensive series of test cases [6]. This paper describes the modules and methods developed to compute the library Bondarenko data for use with ESSM in an assembly lattice physics calculation. A new method is presented to process library Bondarenko data for self-shielding the within-group scatter term of the 2D elastic matrix. The impact of the new processing procedures is demonstrated for lattice physics calculations of several pressurized water reactor (PWR) numerical benchmark cases. Recent developments [7,8] have further improved and extended the capabilities of the original ESSM method, but the library processing methods remain essentially the same.

#### 2.1. AMPX Processing of Bondarenko Data

MG libraries for SCALE are processed with AMPX [9], a modular code system that generates CE and MG cross section data from evaluated nuclear data files such as ENDF/B. AMPX contains modules for a wide variety of functions, including resolved and unresolved resonance processing, Doppler broadening, generation of thermal scattering kernels, and averaging of CE data into MG data. AMPX also includes modules to compute Bondarenko data for self-shielding calculations. A new AMPX module called IRFfactor was recently developed to compute Bondarenko data for ESSM.

To process Bondarenko data, AMPX first computes MG self-shielded cross sections as a function of  $\sigma_0$ , as shown below for the group g, reaction-type x of an arbitrary resonance absorber R, at temperature T:

$$\sigma_{x,g}^{(R)}(\sigma_0,T) = \frac{\int_g \sigma_x^{(R)}(u,T) \,\Phi(u,\sigma_0,T) \,du}{\int_g \Phi(u,\sigma_0,T) \,du},$$
(2.0)

where variable u represents lethargy;  $\sigma_x^{(R)}(u,T)$  is the Doppler broadened CE cross section for reaction type x, and the weighting function  $\Phi(u, \sigma_0, T)$  approximates the fine-structure flux spectrum per unit lethargy for a mixture containing resonance nuclide R at varying degrees of self-shielding, as defined by the value of  $\sigma_0$ . The shielded cross sections are divided by the infinitely dilute values at a reference temperature ( $T_{ref}$ =293K) to obtain f-factors defined by the expression below:

$$f_{x,g}^{(R)}(\sigma_0, T) = \frac{\sigma_{x,g}^{(R)}(\sigma_0, T)}{\sigma_{\infty,g}^{(R)}(T_{ref})}.$$
(2.0)

AMPX provides three options to represent the flux spectrum in eq. (2.1) for computing Bondarenko data in the resolved resonance range: (1) analytical approximation, (2) numerical solution for an infinite homogeneous medium model, and (3) numerical solution for a heterogeneous lattice model. In the unresolved range of all nuclides, f-factors are computed using probability tables whenever data are provided in ENDF.

The analytical approximation uses the following expression based on the intermediate resonance (IR) approximation for the flux per unit lethargy in an infinite homogeneous medium:

$$\Phi(u,\sigma_0,T) = \frac{\sigma_0}{\sigma_t^{(R)}(u,T) + \sigma_0}.$$
(2.0)

Prior to SCALE 6.2, this expression was used to generate Bondarenko data in the resonance range for all library nuclides. However, in processing the ESSM-based SCALE 6.2 libraries, the analytical method is only used in the resolved resonance range to compute Bondarenko data of nuclides with atomic numbers less than zirconium's Z = 40. For heaver nuclides with  $Z \ge 40$ , CE flux spectra are calculated with the SCALE module CENTRM [10] using either a homogeneous or heterogeneous model. CENTRM computes the CE flux spectrum per unit lethargy using an energy mesh typically consisting of 50,000–70,000 energy points, which allows the self-shielded flux to be resolved in great detail.

In the homogeneous model, CENTRM calculates the flux in an infinite medium of an absorber nuclide mixed with hydrogen by solving the following transport equation using CE cross sections:

$$\left(\sigma_{t}^{(R)}(u,T) + \sigma_{0}\right)\Phi(u,\sigma_{0},T) = \int_{u-\varepsilon^{(R)}}^{u} \left(\frac{E}{E'}\right) \frac{\sigma_{s}^{(R)}(u',T)\Phi(u',\sigma_{0},T)}{(1-\alpha^{(R)})} du' + \sigma_{0} \int_{0}^{u} \left(\frac{E}{E'}\right)\Phi(u',\sigma_{0},T) du' + \chi(u), \quad (2.0)$$

where

 $1 - \alpha^{(R)}$  = the maximum fractional energy loss in an elastic collision with absorber nuclide R,  $\varepsilon^{(R)} =$  maximum lethargy gain in an elastic collision =  $\ln\left(\frac{1}{\alpha^{(R)}}\right)$ ,

E, E' = energies corresponding to lethargies u and u', respectively,

$$\sigma_0 = \frac{N^{(H)}}{N^{(R)}} \sigma_p^{(H)}$$
;  $\sigma_p^{(H)}$  = hydrogen potential cross section,

 $N^{(R)}$ ,  $N^{(H)}$  = number densities of nuclide R and hydrogen, respectively, and

 $\chi(u)$  = fission spectrum source term within the fuel mixture.

The purpose of the fission source is to provide a slowing-down spectrum into the resonance range.

The ratio  $\frac{N^{(H)}}{N^{(R)}}$  is varied to obtain the desired set of  $\sigma_0$  values. Library f-factors computed with the analytical flux expression and the CENTRM homogeneous CE spectrum are applied to the 2D heterogeneous lattice physics calculations using homogeneous-heterogeneous equivalence theory.

However, the key feature of ESSM MG library processing is that f-factors in the resolved resonance ranges for designated resonance absorbers are computed from CENTRM CE deterministic calculations of a specified set of *heterogeneous lattice cells*, and they are assigned group-dependent background cross sections based on the same ESSM computational procedure used in the 2D heterogeneous lattice physics calculation. This is described in the next section and is a key difference between the ORNL methodology and that in reference 5.

### 2.2. Computation of ESSM Bondarenko Data Using Heterogeneous Cell Models

The flux spectra used to process Bondarenko data for use with ESSM of a selected absorber nuclide are computed from a set of 2D lattice cells that vary in pitch, moderator density, and absorber concentration so that the desired range of resonance self-shielding is obtained, spanning from infinitely dilute to highly shielded. For each cell, the fuel temperature is also varied according the desired Doppler broadening values. The set of heterogeneous lattices is somewhat arbitrary as long as the lattices cover the full range of resonance shielding conditions for all energy groups. In general, a different set of heterogeneous cells may be required for each resonance absorber. The CENTRM method of characteristics (MoC) solution option [11] is used to compute space-dependent, CE angular flux throughout a given cell; however, the normal procedure for representing the CE cross section data in CENTRM is modified to be consistent with the ESSM assumptions. Because ESSM neglects resonance interference effects between resonance absorbers, the total cross sections of all nuclides in the cell, other than the absorber nuclide of interest, are replaced by the constant potential cross section. Thus, the following equation is used for the CENTRM CE transport calculations of a given 2D cell containing resonance absorber R:

$$\left( \nabla \cdot \Omega + N^{(R)}(r) \sigma_{t}^{(R)}(r, u, T) + \sum_{m \neq R} N^{(m)}(r) \sigma_{p}^{(m)} \right) \Psi(r, u, \Omega; T) = N^{(R)} \int_{E-\varepsilon^{(R)}}^{E} \left( \frac{E}{E'} \right) \frac{\sigma_{s}^{(R)}(u', T) \Phi(r, u', T)}{(1 - \alpha^{(R)})} du' + \sum_{m \neq R} \left\{ N^{(m)}(r) \sigma_{p}^{(m)} \int_{E-\varepsilon^{(m)}}^{E} \left( \frac{E}{E'} \right) \frac{\Phi(r, u', T)}{(1 - \alpha^{(m)})} du' \right\} + \chi(r, u)$$

$$(2.0)$$

The space-dependent flux is averaged over the volume of the resonance absorber to obtain the CE scalar flux spectrum  $\overline{\Phi}(u, \sigma_0^{cell}, T)$ , where  $\sigma_0^{cell}$  is a representative background cross section for the heterogeneous cell. The CE spectrum from CENTRM is passed to the SCALE module PMC [10], which combines it with CE cross section data to compute MG shielded cross sections for the reactions of interest— $\sigma_{x,g}^{(R)}(\sigma_0^{cell}, T)$ —as defined in Eq. (2.1). Eq. (2.2) is used to convert the shielded cross section for the cell into the f-factor,  $f_{x,g}^{(R)}(\sigma_0^{cell}, T)$ . The cell background cross section  $\sigma_0^{cell}$  for each group in the MG library is defined by using the same ESSM procedure applied in the assembly lattice physics calculations.

When applied to self-shielding in an assembly lattice physics calculation, ESSM computes the background cross section in a given group by solving a space-dependent, fixed-source transport equation for the cell geometry. As shown in Williams and Kim, 2012 [1], applying the IR approximation to the scattering sources in Eq. (2.5) and then converting to a MG formulation gives the following set of uncoupled one-group equations for each group g,

$$\nabla \cdot \Omega \Psi_{g}(\mathbf{r},\Omega) + (N^{(R)} \sigma_{a,g}^{(R)} + \Sigma_{p}) \Psi_{g} = \sum_{m} (1 - \lambda_{g}^{(m)}) N^{(m)} \sigma_{p}^{(m)} \Phi_{g}(\mathbf{r}) + \sum_{m} \lambda_{g}^{(m)} N^{(m)} \sigma_{p}^{(m)} , \quad (2.0)$$

where

 $\sigma_{a,g}^{(R)} \rightarrow \sigma_{a,g}^{(R)}(\sigma_0^{cell},T)$  is the self-shielded absorption (i.e., fission + capture) cross section for group g calculated in PMC using the CENTRM CE flux solution for the cell,

$$\sum_{m} \lambda_{g}^{(m)} N^{(m)} \sigma_{p}^{(m)}$$
 is the inhomogeneous source term, and

 $\lambda_g^{(m)}$  is the IR parameter for nuclide m and group g, which is previously computed by another AMPX module.

CENTRM is also used to solve Eq. (2.6) for each heterogeneous cell, and it computes the one-group space-average flux for the mixture containing R. For a given cell, the computed group flux is assumed to be related to the background cross section by the same expression as in Eq. (2.3),

$$\overline{\Phi}_{g}(\sigma_{0}^{cell}) = \frac{\sigma_{0}^{cell}}{\sigma_{a,g}^{(R)} + \sigma_{0}^{cell}},$$
(2.0)

and Eq. (2.7) is solved to obtain the background cross section for the cell:

$$\sigma_0^{cell} = \frac{\sigma_{a,g}^{(R)} \Phi_g(\sigma_0^{cell})}{1 - \Phi_g(\sigma_0^{cell})}.$$
(2.0)

This background cross section expression, also used in subgroup and other similar methods [12,13], can be derived from an equivalence theory approximation for the flux. However, it is important to note that equivalence theory is not used to compute the f-factors, which are obtained from the heterogeneous lattice calculations. The shielded MG cross sections should reproduce the CE values for the selected set of heterogeneous lattice configurations, regardless of the definition of  $\sigma_{0,g}$ , as long as a consistent expression is used in processing the f-factors and in applying ESSM to a lattice. The  $\sigma_0^{cell}$  values computed for the set of heterogeneous lattice cells generally are not uniformly distributed, and some may have similar values for a given group. Therefore, the cell f-factors  $f_{x,g}^{(R)}(\sigma_0^{cell}, T)$  are interpolated to a standardized set of background cross sections (e.g.,  $\sigma_0^{library} = 0.001, 1.0, 10.0, 20.0, 50.0, \dots 10^{10}$ ) for the library tabulation.

The procedure described above for generating ESSM shielding data using heterogeneous cell calculations is automated in the AMPX module called IRFfactor-Het (Intermediate Resonance Ffactors-Heterogeneous option)[9]. IRFfactor-Het is a control module that executes other modules from AMPX and SCALE by calling APIs (application program interface) to compute f-factors and background cross sections using heterogeneous models. A similar module, IRFfactor-Hom, is also available to compute Bondarenko data from homogeneous calculations. Figure 1 shows the flowchart of IRFfactor-Het calculations used to obtain heterogeneous Bondarenko data for ESSM. The SCALE 6.2 package includes several MG libraries based on ENDF/B-VII.1, two of which are mainly for reactor physics applications. These are the 252-group (252g) fine-structure and the 56-group (56g) broad-structure libraries [1]. The 252g library contains Bondarenko data processed using the heterogeneous cell model for the following nuclides: <sup>235</sup>U, <sup>238</sup>U, <sup>239</sup>Pu, <sup>240</sup>Pu, <sup>241</sup>Pu, <sup>91</sup>,Zr, <sup>96</sup>Zr . The 56g library includes heterogeneous Bondarenko data for several additional nuclides contained in PWR AIC control rods: <sup>107</sup>Ag, <sup>109</sup>Ag, <sup>113</sup>In, <sup>115</sup>In, and <sup>113</sup>Cd. In principle, f-factors for any nuclide can be obtained using heterogeneous lattice calculations, but thus far, Bondarenko data for other nuclides can be obtained from homogenous models.

## 2.3. Computation of Self-Shielded Within-Group Elastic Scatter

Historically, Bondarenko self-shielding of the 2D elastic matrix has not been done in SCALE. However, resonance absorption may have an important effect on the elastic removal probability from a group containing one or more resonance, especially for heavy nuclides like <sup>238</sup>U, for which neutrons have a small lethargy gain per elastic collision. Depending on the group width and location of a resonance, absorption reactions can change the fraction of elastic collisions that scatter neutrons out of the group. This is because the group removal probability is largest near the low energy group boundary. This makes the removal and within-group cross sections dependent on self-shielding and Doppler broadening effects, which further changes the group absorption rate. A novel method has been developed for SCALE to address this issue with ESSM, which is not included in other self-shielding methods such as described in reference [5].

The CENTRM transport calculation provides a detailed representation of the CE flux distribution within the group boundaries. Therefore, it is possible to compute the within-group scattering term (i.e., diagonal) of the 2D elastic matrix in a manner similar to that used for other 1D reactions. This procedure is performed by the AMPX IRFfactor module when producing SCALE 6.2 libraries for ESSM self-shielding.



Figure 1. IRFfactor flowchart for computing ESSM self-shielding parameters.

The self-shielded, elastic within-group cross section  $\sigma_{gg}(\sigma_0)$  (i.e., the cross section for a neutron scattering in group g to remain in group g) is given by the expression

$$\sigma_{gg}^{(R)}(\sigma_0) \equiv \frac{\int \sigma_s^{(R)}(u) \ p^{(R)}(u \to g)] \Phi(u, \sigma_0) du}{\int g \Phi(u, \sigma_0) du} , \qquad (2.1)$$

where  $p^{(R)}(u \rightarrow g)$  is the probability that a neutron scattering at lethargy u inside group g will scatter from nuclide R to a higher lethargy contained in group g. In the case of s-wave elastic scatter, this probability is described by a simple analytical expression. The CE flux spectrum in Eq. (2.9) is obtained from a CENTRM transport calculation for a system (either homogeneous or heterogeneous) corresponding to background cross section  $\sigma_0$ . The same ESSM procedures described in the previous section are also used for the within-group Bondarenko data. The shielded cross section in Eq. (2.9) is converted into an f-factor by dividing by the infinitely dilute within-group cross section, which is the diagonal term of the original 2D elastic matrix on the MG library. Hence,

$$f_{gg}^{(R)}(\sigma_0, T) = \frac{\sigma_{gg}^{(R)}(\sigma_0, T)}{\sigma_{gg}^{(R)}}.$$
 (2.2)

The elastic removal cross section  $\sigma_g^{rem}(\sigma_0)$  is the cross section for a neutron scattering in group g to scatter out of the group, which can be computed as the difference in the shielded elastic and within-group cross sections:

$$\sigma_{rem,g}^{(R)}(\sigma_0) \equiv \sigma_{elas,g}^{(R)}(\sigma_0) - \sigma_{g,g}^{(R)}(\sigma_0).$$
(2.3)

The 2D out-scatter terms in the 2D elastic matrix are normalized to sum to the self-shielded removal

$$\sigma_{g \to g'}^{(R)}(\sigma_0) \equiv \frac{\sigma_{rem,g}^{(R)}(\sigma_0)}{\sigma_{rem,g}^{(R)}} \sigma_{g \to g'}^{(R)}, \text{ for } g' > g.$$
(2.3)

#### **3. EXAMPLE RESULTS**

Polaris is a new 2D lattice physics module in SCALE 6.2 that is used for the analysis of light water reactor (LWR) fuel assemblies [6]. Polaris provides MG deterministic-based lattice physics solutions using MoC for the assembly transport calculations and ESSM for self-shielding. The Polaris 2D assembly calculations, the ESSM self-shielding procedures, and the library Bondarenko data processing are integrated in a consistent manner. Polaris uses the SCALE 6.2 252g and 56g libraries with heterogeneous f-factors processed using the procedures described previous sections.

Table 1 shows a comparison of results calculated for several pincell and assembly numerical benchmarks developed for methods comparisons [14]. These cases are similar to a  $17 \times 17$  PWR assembly. Reference results computed with the SCALE 6.2 continuous-energy Monte Carlo code, CE-KENO, are compared to Polaris results calculated using the 252g library with and without the within-group self-shielding factors applied. It can be seen for both pincell and assembly cases that the reactivity discrepancy between KENO and Polaris without self-shielding of within-group cross sections shows a trend to increase as the fuel temperature increases. This is because Doppler broadening affects the probability of scattering out of a group containing a resonance. This behavior led to the development of the methodology described in Section 2.3 for treating elastic removal using f-factors. When within-group f-factors are used in the calculations, the trend is essentially eliminated, and the overall agreement is greatly improved.

**Table 1**. Comparison of CE-KENO and Polaris Results Using ESSM With and Without  $\sigma_{gg}$ . Self-Shielding. (252g library with heterogeneous f-factors)

Benchmark ID	Fuel Temperature (K)	Reference CE-KENO k-eff	<b>Δρ (pcm)</b> NO σ <sub>gg</sub> self-shielding	$\Delta \rho$ (pcm) WITH $\sigma_{gg}$ self-shielding
1b (pin)	600	1.18215	-86	-16
1c (pin)	900	1.17172	-144	-13
1d (pin)	1200	1.16260	-184	2
2b (assembly)	600	1.18336	-100	-37
2c (assembly)	900	1.17375	-146	-28
2d (assembly)	1200	1.16559	-196	-29

In order to examine the effect of using heterogeneous Bondarenko data, a version of the 252g library was processed with no heterogeneous cell calculations for any nuclides (i.e., the library f-factors are computed using CENTRM homogeneous media calculations). Columns 3 and 4 of Table 2 illustrate the impact of using heterogeneous versus homogeneous Bondarenko data in the Polaris ESSM self-shielding for the pincell problem with varying fuel temperatures. The heterogeneous Bondarenko data reduce the homogeneous Bondarenko reactivity bias between CE-Keno and Polaris by about 130 pcm. Neither the homogeneous nor heterogeneous reactivity discrepancies shown in columns 3 and 4, respectively, include within-group self-shielding; and a significant temperature bias is observed in both sets of results. The last column of Table 2 shows the reactivity discrepancy between CE-Keno and Polaris with heterogeneous Bondarenko data when within-group self-shielding is in the ESSM procedure. The temperature bias is eliminated, and there is excellent agreement between Polaris and CE-KENO.

#### 4. SUMMARY

ESSM provides a consistent methodology for processing library Bondarenko data and for performing resonance self-shielding within the context of assembly lattice physics calculations. Bondarenko data for important resonance absorbers on the nuclear data library are processed using CE flux spectra computed for a set of heterogeneous lattice cells for which the background cross sections are defined consistently with the ESSM procedures used in assembly lattice physics calculations. A new approach has been developed to compute Bondarenko data for self-shielding of within-group elastic scattering cross sections with ESSM. New modules have been developed for the AMPX code system to process ESSM Bondarenko data for the MG libraries in SCALE 6.2, and ESSM self-shielding has been incorporated in the SCALE lattice physics code Polaris. Eigenvalues were computed for several numerical benchmarks using Polaris with ESSM and using the SCALE Monte Carlo code CE-KENO. Agreement between results was found to be excellent for all cases. The within-group self-shielding procedure was found to be very effective in reducing observed temperature biases in the reactivity discrepancy. **Table 2.** Comparison of CE-KENO and Polaris Results Computed With Different BondarenkoProcessing Methods:Homogeneous/no  $\sigma_{gg}$  shielding; Heterogeneous/no  $\sigma_{gg}$  shielding , and Heterogeneous/with  $\sigma_{gg}$  shielding. (252g library)

FUEL TEMP (K)	CE KENO $k_{\infty}$	Polaris $\Delta \rho$ (pcm)	Polaris Δρ (pcm)	Polaris Δρ (pcm)
		(Homogeneous,	(Heterogeneous, no	(Heterogeneous,
		no $\sigma_{gg}$ shielding)	$\sigma_{gg}$ shielding)	$\sigma_{gg}$ shielding)
600	1.18539	-235	-114	-19
700	1.18183	-277	-155	-33
800	1.17873	-342	-220	-71
900	1.17497	-323	-200	-26
1000	1.17234	-404	-278	-79
1100	1.16869	-364	-235	-13
1200	1.16593	-400	-267	-24
1400	1.16056	-446	-311	-31
1600	1.15538	-475	-339	-26
1800	1.15042	-495	-360	-19
2000	1.14569	-512	-379	-12
2200	1.14135	-544	-414	-24

#### REFERENCES

- [1] M. L. Williams and Kang-Seog Kim, "The Embedded Self-Shielding Method," PHYSOR 2012, Knoxville, Tennessee (2012).
- [2] B. T. Rearden and M. A. Jessee, Eds., SCALE Code System, ORNL/TM-2005/39, Version 6.2, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2016).
- [3] I. I. Bondarenko, ed., Group Constants for Nuclear Reactor Calculations, Consultants Bureau, New York (1964).
- [4] A. F. Henry, *Nuclear Reactor Analysis*, MIT Press, Cambridge, MA (1982).
- [5] N. Gibson, K. Smith, and B. Forget, "Simple Benchmark for Evaluating Self-Shielding Models," ANS M&C-SNA-MC Conference, Nashville, TN (2015).
- [6] M. A. Jessee et al., "Polaris: A new Two-Dimensional Lattice Physics Analysis Capability for the SCALE Code System," PHYSOR 2014 – The Role of Reactor Physics toward a Sustainable Future, American Nuclear Society, Kyoto, Japan (2014).
- [7] Y. Liu, Y. W. M. Martin, M. L. Williams, and K. S. Kim, "A Full-Core Resonance Self-Shielding Method Using a Continuous-Energy Quasi–One-Dimensional Slowing-Down Solution that Accounts for Temperature-Dependent Fuel Subregions and Resonance Interference," *Nucl Sci Engr 180*, pp 247–272 (2015).
- [8] K. S. Kim, J. Hu, C. A. Gentry, "Embedded Self-Shielding Method Applied to Doubly Heterogeneous Full Ceramic Micro-encapsulated Fuels," submitted to PHYSOR 2016 Conference,

Sun Valley, Idaho (2016).

- [9] D. Wiarda, M. L. Williams, C. Celik, and M. E. Dunn, "AMPX: A Modern Cross-Section Processing System for Generating Nuclear Data Libraries," International Cooperation on Nuclear Criticality Safety (ICNC), Charlotte, NC (Sept.13–15, 2015).
- [10] M. L. Williams, "Resonance Self-Shielding Methodologies in SCALE," Nucl. Technol., 174, 149–168 (May 2011).
- [11] K. S. Kim, M. L. Williams, "The Method Of Characteristics For 2-D Multigroup and Pointwise Transport Calculations in CENTRM," PHYSOR 2012, Advances in Reactor Physics, Linking Research, Industry, and Education, Knoxville, Tennessee (April 15–20, 2012).
- [12] R. J. Stamm'ler et al., HELIOS Methods, Studsvik Scandpower report (1998).
- [13] S. G. Hong and K. S. Kim, "Iterative Resonance Self-Shielding Methods Using Resonance Integral Table in Heterogeneous Transport Lattice Calculations," Ann. Nucl. Energy, 38, 32– 43 (2011).
- [14] A. T. Godfrey, "VERA Core Physics Benchmark Progression Problem Specifications, Revision 4", available online: URL http://www.casl.gov/docs/CASL-U-2012-0131-004.pdf (2014).