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THE EMBEDDED SELF-SHIELDING METHOD

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ABSTRACT

The *embedded self-shielding method* (ESSM) is described for computing resonance-shielded cross sections used in multigroup neutron transport calculations with the SCALE code system. The ESSM "embeds" the self-shielding computation within the transport solution. The transport solution provides information for treating heterogeneous self-shielding effects, and the resulting shielded cross sections are fed back to the transport calculation. Iterations are done to obtain self-consistency. This allows self-shielded cross sections to be generated directly in the transport geometry without requiring external computation of Dancoff factors. The ESSM theory and example calculations are presented.

Key Words: self-shielding, Bondarenko, lattice physics

1. INTRODUCTION

Advanced reactor computational methods used for multidimensional transport calculations provide capability to model complicated systems with explicit representation of most spatial features. However accurate solutions depend on having space-dependent multigroup (MG) cross sections (XS) self-shielded with the local fine-spectrum, which is impacted by non-local heterogeneities. Many self-shielding (S-S) techniques treat these heterogeneous effects through use of a Dancoff factor obtained from a deterministic method-of-characteristics (MoC) or a Monte Carlo calculation for the true multidimensional system. However for full-core computations, more than 10,000 regions may require Dancoff factors. Although some regions may have approximately the same Dancoff factor and may be lumped together, a substantial amount of data and effort is still required.

In this paper we describe a method called the *embedded self-shielding method* (ESSM) that is being developed for the SCALE computation system [1]. The ESSM is fundamentally a variation of the extensively used Bondarenko method [2]; however, it provides tighter coupling between the neutron transport and S-S calculations, so that the heterogeneous S-S effects are consistent with the MG transport calculation of the full system. This is accomplished by embedding the S-S computation within a fixed-source transport calculation that provides scalar fluxes to compute parameters for the Bondarenko method. The fixed-source transport solution can be performed with the same code and geometry used to compute the system eigenvalue, so that shielded XSs are produced directly for the problem-specific transport geometry. In this regard the ESSM is similar to the subgroup approaches in HELIOS [3] and DeCART [4], which use a fixed-source transport solution to compute background XS parameters; however, the proposed method does not require generation of subgroup levels and weights. Instead of solving the transport equation for multiple subgroups, an iterative transport/S-S algorithm is used. A fixed-source transport solution provides parameters for the S-S calculations, and the resulting shielded MG XSs are fed

back to another fixed-source transport calculation, which produces new parameters for the S-S calculation. Iterations are performed to obtain a converged set of self-shielded XSs within a specified tolerance. In principle, the ESSM is quite general and can be used with existing or enhanced 2D or 3D transport solution methods in SCALE [5,6]. The final set of shielded XSs can be used in the eigenvalue transport calculation for the 2D lattice or full-core problem. A recently published paper by Hong and Kim [7] describes an iterative Bondarenko approach—developed independently of this work—which was implemented into a 2D MoC lattice physics code at the Korean Atomic Energy Research Institute (KAERI). Although there are several differences between the KAERI approach and the ESSM, both iterate between the S-S and transport calculations. KAERI shows that results from their iterative method are as accurate as the subgroup method and often run faster [7].

2. DESCRIPTION OF METHOD

The Bondarenko method is based on preprocessing MG data for several different degrees of resonance S-S, as represented by the value of a parameter called the background XS, σ_0. With this method the shielded XS for resonance nuclide "r" is defined as

$$\sigma_{X,g}^{(r)}(\sigma_0^{(r)}) = \frac{\left\langle \sigma_X^{(r)}(E)\, \varphi(E;\sigma_0^{(r)}) \right\rangle_g}{\left\langle \varphi(E,\sigma_0^{(r)}) \right\rangle_g} , \quad (1)$$

where $\varphi(E;\sigma_0^{(r)})$ is the fine-spectrum for a system characterized by the background XS $\sigma_0^{(r)}$. As part of future development efforts for SCALE, the preprocessed shielded data will ultimately be obtained from a series of CENTRM [8]calculations for heterogeneous unit cells with varying pitch and/or moderator densities that span the desired range of $\sigma_0^{(r)}$ values as defined by lattice equivalence theory. However, the initial approach described here computes the flux fine-spectrum using CENTRM pointwise (PW) slowing-down calculations for an infinite homogeneous medium containing the resonance material mixed with hydrogen with varying concentration ratios that produce the desired range of $\sigma_0^{(r)}$ values, where the background XS for this system is $\sigma_{0,g}^{(r)} = \frac{N^{(H)}}{N^{(r)}}\sigma_{p,g}^{(H)}$. The calculated PW spectra $\varphi(E;\sigma_0^{(r)})$ from CENTRM are used to evaluate eq. (1) for the specified background XSs, and the resulting shielded MG values are stored on the SCALE nuclear data libraries.

The Bondarenko method uses the second equivalence theorem to relate the preprocessed shielded values for homogeneous systems to actual reactor configurations. This approach defines a background XS for an equivalent homogeneous system that produces (nearly) the same resonance integral as a heterogeneous system. For a given spatial region Z containing a single mixture within a heterogeneous system, the macroscopic background XS for an equivalent homogeneous system is usually defined in the conventional Bondarenko method as

$$\Sigma_{0,g}^{(Z)} = \sum_{j \in Z} \lambda_g^{(j)} \Sigma_p^{(j)} + \Sigma_{esc}^{(Z)} . \quad (2)$$

In this expression, $\lambda_g^{(j)}$ are group-dependent intermediate resonance (IR) parameters; $\Sigma_p^{(j)}$ and $N^{(j)}$ are the potential XS and number density of moderating nuclide *j*, respectively; and the escape XS $\Sigma_{esc}^{(Z)}$ is a function of the dimensions and shape of zone Z as well as the Dancoff factor. The system Dancoff factor may be quite difficult to determine for complex heterogeneous cores with many non-uniformities. SCALE has the capability to compute this quantity using Monte Carlo, but this requires an auxiliary calculation. One of the major advantages of the ESSM is that it avoids the need to compute a Dancoff factor.

The following analytical approximation for the MG flux in region Z can be obtained by applying the IR approximation to the equivalence theory expression for the flux in group g with lethargy width of Δu_g [8]:

$$\Phi_g^{(Z)} = \frac{\Sigma_{0,g}^{(Z)} \Delta u_g}{\left\{\Sigma_{a,g}^{(Z)} + \left(\lambda\Sigma_{s,g}^{(Z)} - \lambda\Sigma_{p,g}^{(Z)}\right) + \Sigma_{0,g}^{(Z)}\right\}} \quad . \tag{3}$$

In the above expression, the short-hand notation is introduced such that $\lambda\Sigma_{s,g}^{(Z)} \equiv \sum_{j \in Z} \lambda_g^{(j)} \Sigma_{s,g}^{(j)}$; and $\lambda\Sigma_{p,g}^{(Z)}$ is defined similarly. Conversely, if the MG flux is known, eq. (3) can be solved for the macroscopic background XS in region Z,

$$\Sigma_{0,g}^{(Z)} = \frac{\Sigma_{a,g}^{(Z)} \Phi_g^{(Z)} + \lambda\left(\Sigma_{s,g}^{(Z)} - \Sigma_{p,g}^{(Z)}\right)\Phi_g^{(Z)}}{\Delta u_g - \Phi_g^{(Z)}} \quad . \tag{4}$$

The microscopic background XSs for resonance nuclide *r* is defined as $\sigma_{0,g}^{(r)}(Z) = \frac{\Sigma_{0,g}^{(Z)} - \lambda_g^{(r)}\Sigma_p^{(r)}}{N^{(r)}}$, and the shielded XS is obtained by interpolating the pre-processed tabulated values to this $\sigma_{0,g}^{(r)}(Z)$ value.

In the ESSM method the region-averaged MG flux appearing in eq. (4) is computed by solving the multidimensional transport equation, using the IR approximation for the scattering source in order to be consistent with the analytical flux expression in eq. (3). As shown in reference [9], this equation corresponds to

$$\nabla \cdot \Omega \Psi_g(r,\Omega) + \Sigma_{t,g}^{(Z)} \Psi_g(r,\Omega) = (1-\lambda)\Sigma_{s,g}^{(Z)} \Phi_g(r) + \lambda\Sigma_{p,g}^{(Z)} \Delta u_g \ . \tag{5}$$

Equation (5) is a MG transport equation with a region-dependent inhomogeneous source of $(1\text{-}\lambda)\Sigma_p^{(Z)} \Delta u_g$, which can be solved with existing transport solvers in SCALE. The computed angular flux $\Psi_g(r,\Omega)$ is integrated over direction and averaged over region Z to obtain $\Phi_g^{(Z)}$ for later use in the S-S calculation.

To solve the MG transport equation, self-shielded XSs for every region Z are required. The shielded XSs are computed using the Bondarenko method as described previously. Since self-

shielded XSs depend on fluxes obtained from the transport calculation, an iterative procedure must be employed to converge the values of the shielded XSs and fluxes [9]. The fixed-source transport calculations for each group, as well as the S-S computations for each spatial region, are independent, so they may be done in parallel. Figure 1 shows the iterative scheme being used. The entire algorithm is completed prior to performing the eigenvalue transport calculation, so the ESSM procedure can be modularized.

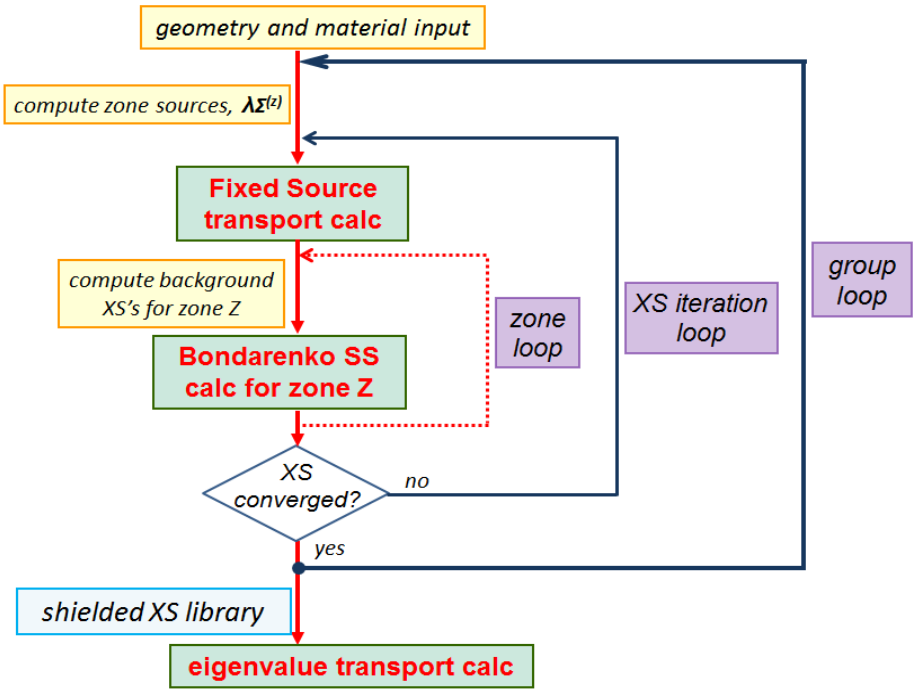

Figure 1. ESSM iterative procedure.

3. RESULTS

A typical fuel pin of a pressurized water reactor (PWR) has been selected as an initial sample problem to test the ESSM. Geometry and composition data for the sample problem are shown in Table I. The reference solution was obtained by performing an MCNP calculation with reflecting boundary conditions, using ENDF/B-VII.0 continuous energy (CE) cross sections.

Two SCALE calculations were performed for the sample problem using the NEWT 2-D discrete ordinates lattice physics code. The first SCALE/NEWT calculation used 238-group ENDF/B-VII.0 cross sections that were self-shielded by the BONAMI/CENTRM/PMC modules in SCALE. The CENTRM calculation to obtain self-shielded 238-group cross sections was performed for a 1-D Wigner-Seitz cylindrical pin configuration using the discrete ordinate (S_N) method, with a pointwise energy mesh of approximately 50,000 points. The second SCALE/NEWT calculation used 81-group ENDF/B-VII.0 cross sections that were self-shielded by BONAMI/CENTRM/PMC. However, the CENTRM pointwise transport calculation was performed using a new 2-D MoC [10] option and a square pin configuration similar to the MCNP model. The 81-group cross sections were processed from a new SCALE 81-group library [11].

Table I. PWR pincell geometry and composition

Region	Material	Temperature (K)	Radius, pitch (cm)	Density (g/cm^3)
Fuel	UO_2	600	0.4025	10.4
Clad	^{27}Al	600	0.4759	2.7
Moderator	H_2O	600	0.7120 (1.2620)	0.65

Self-shielded cross sections computed with the ESSM module were used in a MoC transport solver to obtain the eigenvalue for the sample problem. The 81-group library was used for these calculations, in which the Bondarenko factors as a function of background cross sections were prepared from the CENTRM pointwise transport calculations for a homogeneous model.

It was found that the ESSM computation converged in three iterations for this case. Figure 2 provides a comparison of neutron spectra obtained from the MCNP, NEWT, and ESSM eigenvalue calculations. As shown in Fig. 2, the neutron spectrum from ESSM is very consistent with the neutron spectra from the other codes in the energy range below 20 keV where the method was applied. Variations in the high energy range are caused by group structure differences in representing the fission spectrum, which is not related to the ESSM. Table II provides a comparison of eigenvalues calculated by the various codes. The ESSM eigenvalue agrees within the statistical uncertainty of MCNP, and is even slightly better than the result obtained with NEWT using the continuous-energy self-shielding method in CENTRM. The computational result shows that the newly developed ESSM module is working well.

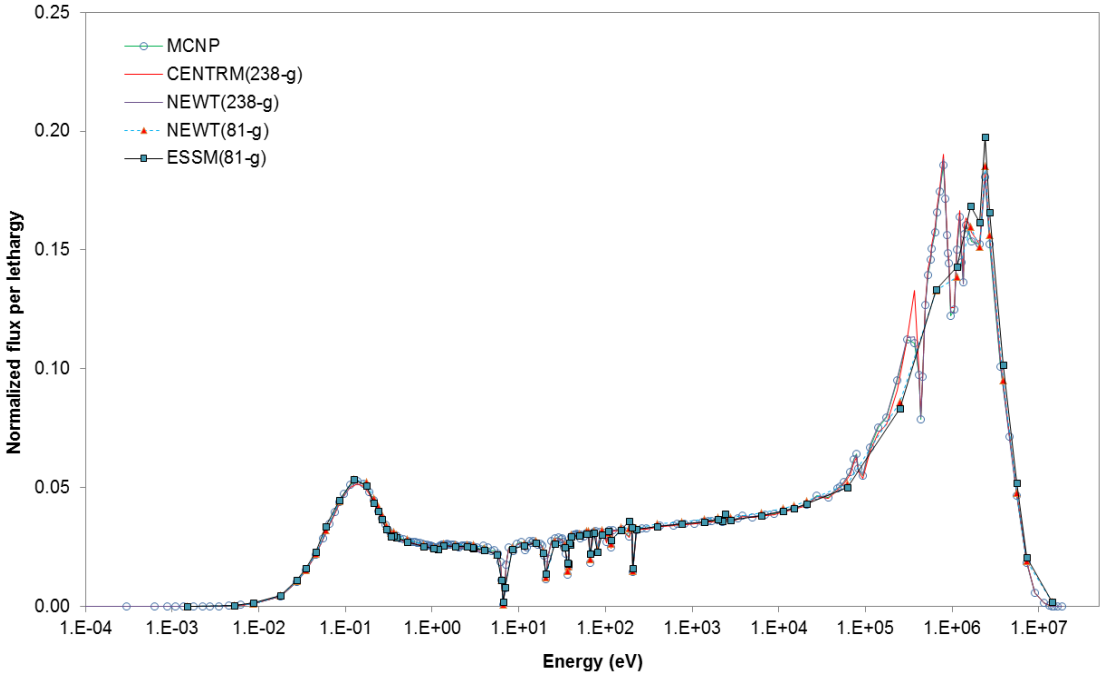

Figure 2. A comparison of neutron spectra.

Table II. A comparison of eigenvalues for PWR pincell

Code	Multiplication factor	Δρ (pcm)
MCNP	1.3736 ±0.00013	-
CENTRM(S_N)/NEWT (238-g)	1.36744	325
CENTRM(MoC)/NEWT (81-g)	1.37011	183
ESSM/MoC (81-g)	1.37323	17

4. SUMMARY

The ESSM provides an improved method for Bondarenko S-S which accounts for the impact of multidimensional heterogeneous effects without requiring an independent Dancoff factor calculation. Similar to the subgroup approach, a fixed-source, multidimensional transport calculation is performed to obtain region-averaged MG fluxes for computing the background XS in the S-S operations. However, no subgroup levels are used. Instead, iteration between the S-S and transport solutions is done to obtain consistent self-shielding and transport solutions. This makes the ESSM method easy to implement in existing Bondarenko-based lattice physics codes. Results show that the iterative procedure converges rapidly and produces accurate results. This method is currently being incorporated into a new SCALE lattice sequence.

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