Preliminary Assessment of Resonance Interference Consideration by Using 0-D Slowing Down Calculation in the Embedded Self-Shielding Method*

Kang-Seog Kim and Mark L. Williams

Oak Ridge National Laboratory: 1 Bethel Valley Rd., P.O. Box 2008, Oak Ridge, Tennessee 37831
kimk1@ornl.gov; williamsml@ornl.gov

INTRODUCTION

The embedded self-shielding method (ESSM) [1] has been developed to estimate the local self-shielded cross sections (XS) for the SCALE computation system [2]. The ESSM is fundamentally a variation of the extensively used Bondarenko method [3]; however it provides tighter coupling between the neutron transport and self-shielding(S-S) calculations, so that the heterogeneous S-S effects are consistent with the multi-group (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. However, this ESSM includes a drawback in resonance interference consideration which is achieved by the Bondarenko iteration.

In SCALE 6, resonance interfered self-shielded cross sections are obtained by solving a slowing down equation for a heterogeneous pin cell. [4] Although this approach is able to consider resonance interference explicitly, the computing time is very expensive and the accuracy for a multi-pin problem is dependent upon a quality of Dancoff factor.

It is known that interference between resolved resonances is not sensitive to the environment, [5] which enables resonance interference correction terms to be obtained from 0-D slowing down calculations equivalent to the heterogeneous model. The purpose of this paper is to assess the possibility of coupling of ESSM with a 0-D slowing down calculation equivalent to the heterogeneous model in which basis self-shielding calculations are performed by ESSM and resonance interference corrections are made by 0-D slowing down calculation, and to setup the overall procedure in the SCALE system.

DESCRIPTION OF METHOD

A new procedure of ESSM coupled with 0-D slowing down could be established through various slowing down analyses in the following section as follows.

a. Self-shielded cross sections for each nuclide are obtained by solving the following pointwise slowing down equation without any resonance interference for 2-D pin cell configuration.

$$\hat{\Omega}\cdot\nabla\psi_k + \sum_i \Sigma_{i,t}^k(u)\psi_k(u,\hat{\Omega}) = \sum_i \int_{u-\Delta_i}^{u} \Sigma_{i,s}^k(u')\phi_k(u')\frac{\exp(u'-u)}{1-\alpha_i}du', \tag{1}$$

where

$$\begin{aligned} &\Sigma_{i,x} = N_i\sigma_{i,x}, \\ &\Sigma_{i,s}^k(u) = \Sigma_{i,p}^k + \Sigma_{i,rs}^k(u), \\ &\Sigma_{i,t}^k(u) = \Sigma_{i,s}^k(u) + \Sigma_{i,ra}^k(u), \\ &\alpha_i = (A_i-1)^2/(A_i+1)^2, \\ &\Delta_i = -\ln(\alpha_i). \end{aligned} \tag{2}$$

In eq. (1), $\Sigma(u)$ and N are the total macroscopic cross section and atomic number density, respectively and A_i and Δ_i are the atomic mass and the maximum lethargy gain per collision with isotope i, respectively. 1-α_i is the maximum fractional energy loss per collision with isotope i. The pointwise scalar flux can be obtained by solving eq. (2) using the pointwise cross sections. The effective self-shielded cross section of the resonance isotope for each group can be obtained by using the following equation:

$$\sigma_{x,g} = \frac{\int_{\Delta u_g}\sigma_x(u)\phi(u)du}{\int_{\Delta u_g}\phi(u)du}. \tag{3}$$

In eq. (1) only one resonance nuclide is considered to exclude resonance interference and other nuclides are treated as background nuclides including only potential scattering cross section.

b. The corresponding background cross section is calculated by using the following ESSM equations for the same pin cell configuration.

$$\hat{\Omega}\cdot\nabla\psi_{g,k} + \sum_i \Sigma_{i,g,t}^k\psi_{g,k}(\hat{\Omega}) = \sum_i \lambda_{i,g}\Sigma_{i,p}^k + \sum_i (1-\lambda_{i,g})\Sigma_{i,g,s}^k\phi_{g,k}. \tag{4}$$

*Notice: This manuscript has been authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes.

$$\sigma_{g,b} = \frac{\Sigma_{g,b}}{N_R} = \frac{\sum_i N_i \lambda_i \sigma_{i,g,p} + \Sigma_{g,e}}{N_R} = \frac{\sigma_{g,a}\phi_g}{1-\phi_g} \ . \qquad (5)$$

c. Full Bondarenko F-factors as a function of background cross section can be generated by changing dilution (composition and geometry) which are called heterogeneous F-factors.

d. In the application eq. (4) is solved for any geometrical configuration and the background ($\sigma_{g,b}$) and equivalence cross sections ($\Sigma_{g,e}$) can be obtained by using eq. (5). Basis self-shielded cross sections ($\tilde{\sigma}_{i,x,g}$) can be read from the heterogeneous F-factor table.

e. Conventionally resonance interferences are considered through the Bondarenko iteration. However, in the new procedure resonance interference terms are obtained by solving the following slowing down equation equivalent to the heterogeneous problem in which equivalence cross section ($\Sigma_{g,e}$) is from eq. (5).

$$(\sum_i \Sigma_{i,t}^k(u) + \Sigma_{g,e})\psi_k(u,\hat{\Omega}) = \sum_i \int_{u-\Delta_i}^{u} \Sigma_{i,s}^k(u')\phi_k(u')\frac{\exp(u'-u)}{1-\alpha_i}du' + \Sigma_{g,e} \ . \qquad (6)$$

Resonance interference terms can be obtained from two different homogeneous calculations. All the resonance nuclides are included in the first calculation (interfered) and only one target resonance nuclide is considered in the second calculation (non-interfered). Resonance interference correction terms can be calculated by using the following equation.

$$\Delta\hat{\sigma}_{i,x,g} = \hat{\sigma}_{i,x,g}^{interfered} - \hat{\sigma}_{i,x,g}^{noninterfered} \ . \qquad (7)$$

f. Final self-shielded cross sections will be as follows:

$$\sigma_{i,x,g} = \tilde{\sigma}_{i,x,g} + \Delta\hat{\sigma}_{i,x,g} \ . \qquad (8)$$

If there are N resonance nuclides at the step "e," the computing time will be very expensive because N+1 0-D slowing down calculations should be performed to obtain resonance interference terms for each nuclide. In order to avoid this computational burden, other Bondarenko F-factors based on homogeneous model should be provided for each nuclide which are called homogeneous F-factors. In this case only one interfered 0-D slowing down calculation will be required. Since the equivalence cross section ($\Sigma_{g,e}$) is provided from ESSM, the effective self-shielded XSs without resonance interference can be read from the homogeneous F-factor table. The only problem in this method is that the AMPX master library or other library for transport lattice codes should include two types of Bondarenko F-factors based on heterogeneous and homogeneous models.

ANALYSIS AND RESULTS

A typical PWR fuel pin cell with UO_2 fuel has been selected for analysis. When considering resonance interference effect, pointwise cross sections for both U^{235} and ^{238}U are included. When disregarding resonance interference, one of two resonant nuclides (^{235}U and ^{238}U) is treated as background nuclide which includes only potential cross section.

Importance of resonance interference

Figures 1 and 2 provide comparisons of interfered and non-interfered self-shielded absorption and fission cross sections for ^{235}U and ^{238}U. As shown, there are large differences in XSs for several resonance groups. Typically these resonance interferences are treated by the Bondarenko iteration. However, they cannot be effectively considered due to the complicated resonance shapes, which results in a discrepancy in reaction rate and eigenvalue.

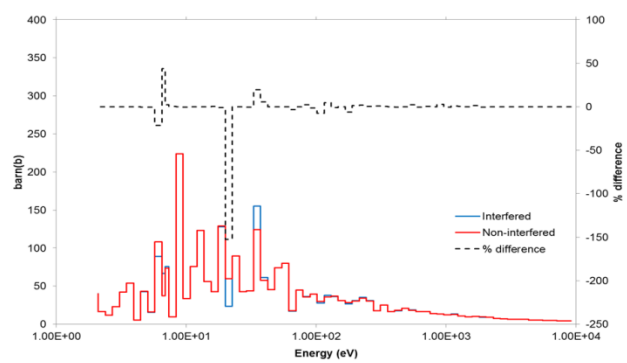

Fig. 1. A comparison of interfered and non-interfered self-shielded cross section (^{235}U absorption)

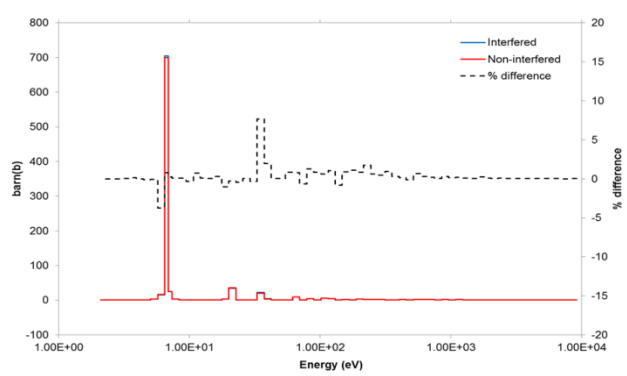

Fig. 2. A comparison of interfered and non-interfered self-shielded cross section (^{238}U absorption)

Sensitivity to environment

To determine how sensitive resonance interference is to the environment, two different pin configurations were selected. The first one was a typical PWR fuel pin, and the second one included a 50% void in the moderator. Slowing down calculations for two fuel pins were performed with and without resonance interference. Resonance interference terms were calculated for each pin, and fractional differences between resonance interference terms for two pins were calculated, and compared to the fractional resonance interference terms. The sensitivities of interfered self-shielded absorption cross sections to environment for ^{235}U and ^{238}U are shown in Figures 3 and 4, respectively.

As can be noted, the resonance interference terms are insensitive to environment, indicating that a new procedure would be much simpler. In other words, it is probable that resonance interference terms for a heterogeneous model can be accurately generated from a simplified homogeneous model.

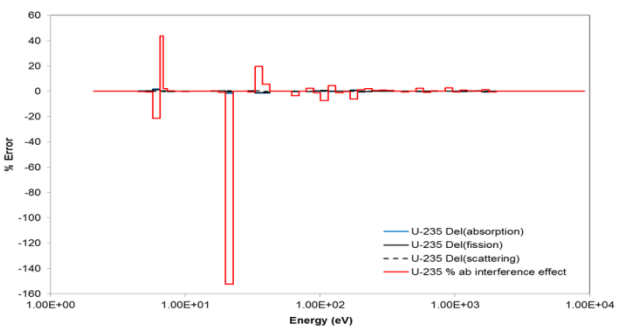

Fig. 3. Sensitivity of interfered self-shielded cross section to environment (^{235}U)

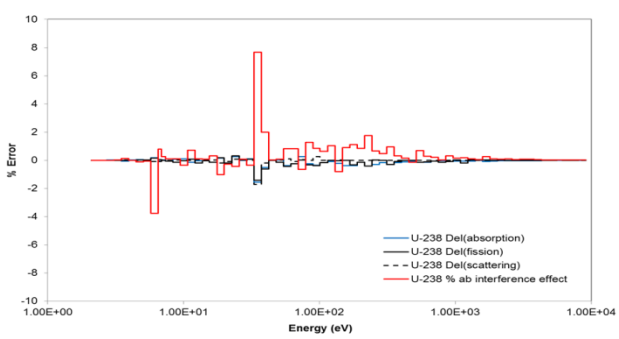

Fig. 4. Sensitivity of interfered self-shielded cross section to environment (^{238}U)

Homogeneous vs. heterogeneous models

Any differences between self-shielded cross sections from homogeneous and heterogeneous models must be determined. The equivalence cross sections ($\Sigma_{g,e}$) for fuel region are obtained from the heterogeneous model by using eqs. (1), (4) and (5), and then eq. (6) is solved with $\Sigma_{g,e}$ from the heterogeneous calculation. Since both cases provide the same background cross section, a comparison of self-shielded cross sections provides the difference between homogeneous and heterogeneous models in self-shielded cross sections.

Figures 5 and 6 provide absolute and fractional differences between self-shielded cross sections from homogeneous and heterogeneous models for ^{235}U and ^{238}U, respectively. While there are relatively small differences in ^{235}U, there are significant differences in ^{238}U. This result shows why the heterogeneous F-factors should be used as the basis self-shielded XSs instead of homogeneous F-factors.

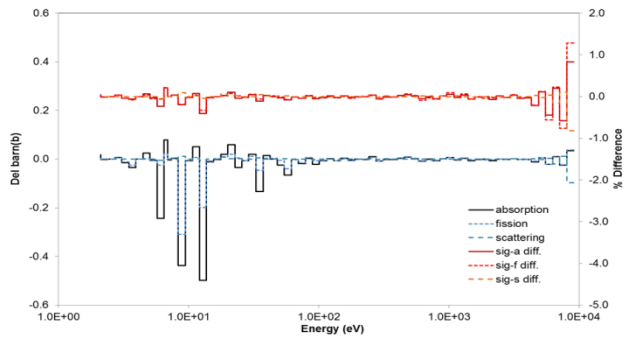

Fig. 5. A comparison of self-shielded cross sections (homogeneous vs. heterogeneous, ^{235}U)

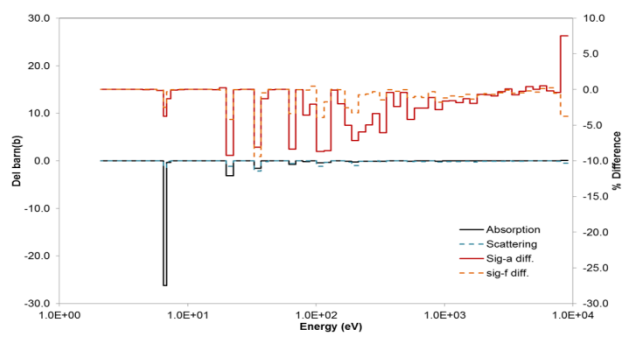

Fig. 6. A comparison of self-shielded cross sections (homogeneous vs. heterogeneous, ^{238}U)

Accuracy of 0-D resonance interference

Although it was shown that the resonance interference effect is not sensitive to environment, the effectiveness of resonance interference terms obtained from 0-D slowing down calculation in heterogeneous models must still be determined. Resonance interference terms for heterogeneous models are directly obtained from slowing down calculations using eq. (1), from which the equivalence cross sections ($\Sigma_{g,e}$) for fuel region are obtained using eqs. (4) and (5). Then eq. (6) is solved with $\Sigma_{g,e}$ from the heterogeneous calculation from which resonance interference terms are obtained.

Figures 7 and 8 provide fractional differences between resonance interferences from the homogeneous and heterogeneous models for ^{235}U and ^{238}U. In order to see how small these differences are, they are compared to the fractional differences in self-shielded absorption cross sections due to resonance interferences. It is noted that resonance interference terms from the 0-D slowing down calculation are very consistent with the heterogeneous ones.

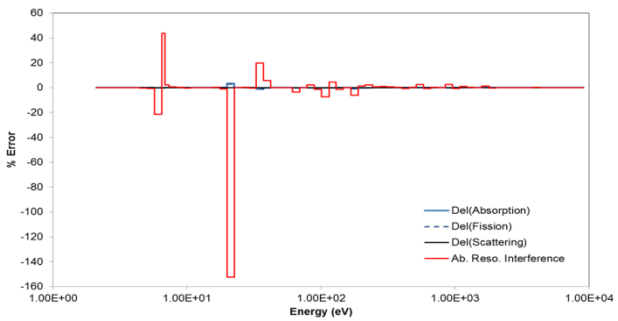

Fig. 7. A fractional difference of self-shielded cross sections from homogeneous and heterogeneous models (^{235}U)

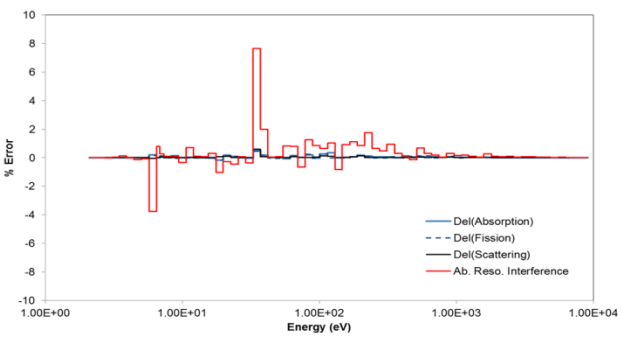

Fig. 8. A fractional difference of self-shielded cross sections from homogeneous and heterogeneous models (^{238}U)

CONCLUSION

Figure 9 provides a diagram of ESSM with resonance interference treatments based on the Bondarenko iteration method or the 0-D slowing down calculation in the AMPX [6] and SCALE code systems. Computing time for a 1 million group 0-D slowing down calculation with equivalent lethargy width is less than 0.2 sec, which is not a burden and can be easily parallelized. In addition, there is room to improve computing time by using a non-equivalent lethargy width.

This procedure is promising for the next-generation transport lattice code which includes the advantages of the SCALE-BONAMI/CENTRM approach for the explicit resonance interference and various Bondarenko approaches such as ESSM and the subgroup methods to estimate self-shielded XSs considering the problem-specific geometry.

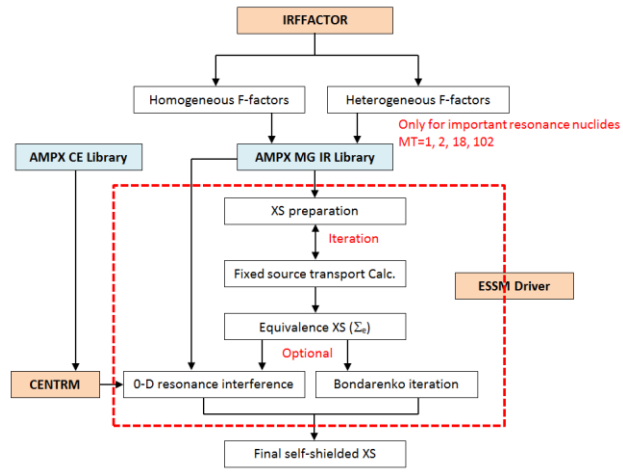

Fig. 9. Flow chart of a new resonance interference treatment

REFERENCES

1. Mark L. Williams, Kang-Seog Kim, "The Embedded Self-Shielding Method," PHYSOR 2012, Knoxville, Tennessee, USA, April 15-20, 2012.
2. SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design, ORNL/TM-2005/39, Version 6.1, June 2011. (Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-785.)
3. I. I. Bondarenko, "Group Constants for Nuclear Reactor Calculations," Consultants Bureau, New York (1964).
4. Mark L. Williams, "Resonance Self-Shielding Methodologies in SCALE 6," *Nuclear Technology*, **174**, 149-168 (2011).
5. Mark L. Williams, "Correction of Multigroup Cross Sections for Resolved Resonance Interference in Mixed Absorbers," *Nucl. Sci. Eng.*, **83**, 37-49 (1983).
6. M. E. Dunn and N. M. Greene, "AMPX-2000: A Cross-Section Processing System for Generating Nuclear Data for Criticality Safety Applications," *Trans. Am. Nucl. Soc*. **86**, 118–119 (2002).