Transactions of the Korean Nuclear Society Autumn Meeting
Pyeongchang, Korea, October 30-31, 2014

Improvement of Resonance Interference Treatment in STREAM

Sooyoung Choi, Azamat Khassenov, and Deokjung Lee*

Ulsan National Institute of Science and Technology, UNIST-gil 50, Eonyang-eup, Ulju-gun, Ulsan, 689-798, Korea
*csy0321@unist.ac.kr, azamat@unist.ac.kr and deokjung@unist.ac.kr**
**Corresponding Author*

1. Introduction

The MOC neutron transport code STREAM has been developed in UNIST [1]. Equivalence theory [2] has been adopted as a resonance treatment method in STREAM. Equivalence theory is widely used in production calculations to calculate effective multigroup (MG) cross-sections (XS) for commercial reactors. Although a lot of methods have been developed to enhance the accuracy in computing effective XSs, the current resonance treatment methods, including equivalence theory, still do not have a clear resonance interference model.

The conventional resonance interference model simply adds the absorption XSs of resonance isotopes to the background XS [2]. The Bondarenko iteration method performs iteration on it till effective XSs converge [2, 3]. However, the conventional models are not enough to consider the interference effects, which results in non-negligible errors in computing effective XSs. The conventional methods assume that the absorption XSs are flat within an energy group, but the resonance interference occurs complicatedly within a coarse MG, therefore a way to solve this problem is to increase the number of resonance energy groups sufficiently, such as with the ultra-fine group (UFG) method. Recently research has been performed on UFG methods which solve the slowing down equation and then calculate the MG XS or the correction factor [4], but the UFG transport calculations cannot be practically used due to limited computing capacity. In addition, there are still problems such as geometric limitations and long computation time.

In this paper, a new practical resonance interference method is presented which uses the resonance interference factor (RIF) method [4-6]. However, unlike the original RIF method, this new method interpolates the RIFs in a pre-generated RIF library and corrects the effective XS, rather than solving the time consuming slowing down calculation. The new RIF method and conventional resonance interference methods have been implemented and compared in STREAM. The verification results using the proposed method show significant improvements of accuracy in treating the interference effect.

2. Methodology

2.1 Conventional Resonance Interference Models

The conventional equivalence theory [2] computes the effective XS first by assuming that only a target resonance isotope has an absorption XS, and other isotopes have potential scattering XSs. After the XSs of all isotopes in a fuel material are computed, the effective XS of the target isotope is re-evaluated by summing the absorption XSs of the other resonance isotopes into its background XS as follows:

$$\sigma_a^i = \frac{RI_a^i\left(\sigma_b^i + \bar{\sigma}_a\right)}{1 - RI_a^i\left(\sigma_b^i + \bar{\sigma}_a\right)\Big/\left(\sigma_b^i + \bar{\sigma}_a\right)} , \qquad (1)$$

where RI_a^i is the absorption resonance integral, σ_b^i is the background XS, σ_a^i is the absorption XS of isotope *i*, and $\bar{\sigma}_a$ is an absorption XS of other resonance isotopes which is defined by:

$$\bar{\sigma}_a = \frac{1}{N^i}\sum_{j\neq i} N^j \sigma_a^j . \qquad (2)$$

The Bondarenko iteration method [2, 3] is similar to the conventional resonance interference method. However, this method evaluates the effective XSs till the XSs converge. 3 ~ 4 iterations make it converge.

2.2 New RIF Library Method

The RIF method [4-6] computes UFG flux spectrums by solving the slowing down equation for each of the isolated resonance absorbers and the fuel mixture as a whole, and generates the resonance interference correction factor using Eq. (3).

$$f_{x,g}^r = \frac{\sigma_{x,g}^{r,\mathrm{mix}}}{\sigma_{x,g}^{r,\mathrm{iso}}} = \frac{\sum_{u\in g}\sigma_{x,u}^{r,\mathrm{mix}}\phi_u^{\mathrm{mix}}\Big/\sum_{u\in g}\phi_u^{\mathrm{mix}}}{\sum_{u\in g}\sigma_{x,u}^{r,\mathrm{iso}}\phi_u^{\mathrm{iso}}\Big/\sum_{u\in g}\phi_u^{\mathrm{iso}}} , \qquad (3)$$

where x is the reaction type, g is the group index of MG, u is the group index of UFG, and r is index for the resonance absorber.

The RIF is used to correct the effective XS to consider the resonance interference effect using Eq. (4).

$$\hat{\sigma}^r_{x,g} = f^r_{x,g}\sigma^r_{x,g} \ , \qquad (4)$$

where $\sigma^r_{x,g}$ is the effective XS generated by equivalence theory and $\hat{\sigma}^r_{x,g}$ is the corrected effective XS by RIF.

In the new RIF library method, RIFs are pre-generated as with the MG library. The RIFs are computed in a homogeneous system for various background XSs, energy groups, reaction types, temperatures, and atom ratios of resonance absorbers. A UFG slowing down code has been written and used to generate the library.

If the number of resonance isotopes increases as burnup increases, the number of combinations of resonance isotopes increases dramatically. In that case, the size of the RIF library can be a problem. Therefore, in this RIF library method, interaction between two resonance isotopes are considered, and the interference effect of more than two resonance absorbers is approximated by the sum of each interference effect. The interference correction method with the RIF library is described as follows:

1) Compute the effective XS $\sigma^r_{x,g}$ by equivalence theory or another method without considering the resonance interference effects. r is a resonance isotope to be corrected.
2) Interpolate RIF $f^{r\leftarrow k}_{x,g}$ into the RIF library with the background XS, and the atom ratio. $f^{r\leftarrow k}_{x,g}$ is a RIF considering the interference effect from isotope k to target isotope r.
3) Compute perturbations of the effective XSs from the interference effect of isotope k using Eq. (5)

$$\Delta\sigma^r_{x,g} = \sum_{k\in\text{Fuel}} \left[\sigma^r_{x,g}\left(f^{r\leftarrow k}_{x,g} - 1\right)\right] . \qquad (5)$$

4) Add the perturbation term into the effective XS using Eq. (6)

$$\hat{\sigma}^r_{x,g} = \sigma^r_{x,g} + \Delta\sigma^r_{x,g} \ . \qquad (6)$$

5) Perform procedures 1) ~ 4) for all resonance isotopes in the RIF library.

The RIF correction is performed for absorption, fission, and scattering XSs, and all resonance energy groups.

3. VERIFICATION

3.1. Description Verification Problem

A homogeneous U/H medium was modeled to eliminate the bias from the heterogeneous effect. Rather than solving the heterogeneous problem, ^{1}H was filled to set the background XS of ^{238}U to be 50 ~ 60 barn, which is a typical value for a PWR. The initial enrichment of the fuel is 5 wt% and the fuel was depleted to 60 MWd/kgU burnup. The depletion calculation was performed by CASMO4E. The material composition of each burnup step was saved and used as inputs of MCNP6 and STREAM. Therefore there is no material composition difference between MCNP6 and STREAM for each burnup step. The number of isotopes considered in the depletion chain is more than 63 including U, Pu, Am, and fission products. Lumped fission products from CASMO4E results are ignored. In the RIF method, the interference effect among 40 resonance isotopes (*i.e.* U, Pu, Am, Rh, Xe, Cs, and Sm) are considered

3.2. Verification Results

The problem was solved by STREAM. In the STREAM calculation, 4 kinds of resonance interference methods were tested.

1) STREAM (ignored) : The resonance interference effect is ignored.
2) STREAM (Conv.) : The conventional resonance interference model described in Eq. (1).
3) STREAM (Bon.iter.) : The Bondarenko iteration method.
4) STREAM (RIF): The new RIF library method proposed in this paper.

The STREAM results were compared to MCNP6. The eigenvalue results and error of the STREAM results are shown in Figs. 1 and 2, respectively. In Fig. 2, the error was calculated as an eigenvalue difference compared to MCNP6 and the unit is pcm. The standard deviation of MCNP6 results is 6 ~ 7 pcm for each burnup step.

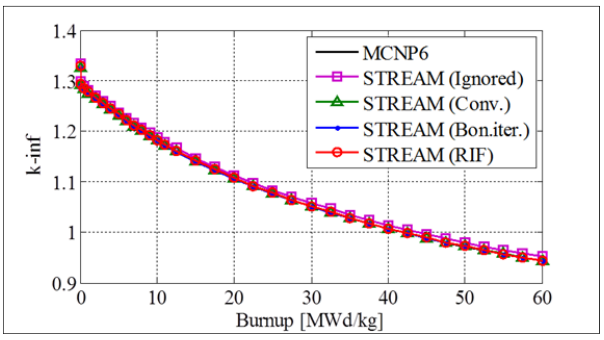

Fig. 1. Eigenvalue calculation results as burnup steps.

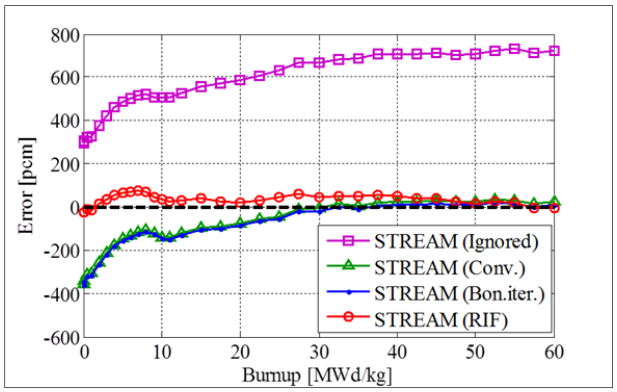

Fig. 2. Error of eigenvalue compared to MCNP6.

If the resonance interference effect is ignored, STREAM (ignored) shows more than 300 pcm of error for all burnup steps and about 700 pcm error for 60 MWd/kgU burnup.

The conventional resonance interference method and the Bondarenko iteration method show an average of 600 ~ 700 pcm lower results than when the interference is ignored, and the results of the two methods (Conv. and Bon.iter.) are close to each other. The difference between the two methods is less than 20 pcm for all burnup steps. In the initial step, the two methods have about 350 pcm of error and the error decreases as burnup increases, however, these behaviors are error cancelation results among complicated resonance interference effects. It will be treated in more detail in a following session.

The new RIF library method shows the most accurate results compared to the other three methods. The RIF method shows less than 100 pcm of error for all burnup steps. The maximum error of the RIF method is 73 pcm at 7 MWd/kgU burnup. Elapsed time for the RIF library method can be ignored because several simple interpolation calculations are performed. Therefore it can be said that the RIF methods treats the resonance interference exactly and shows promise to be used for practical calculations.

3.3 Comparison of Reaction Rate.

In the previous sections, the conventional method and the Bondarenko iteration method seem to give accurate results as burnup increases. A detailed reaction rate comparison was performed to confirm whether it is an error cancelation effect or not. The nu-fission reaction rate is normalized to 1, therefore the absorption reaction rate difference presents an error of eigenvalue for corresponding isotopes and energy groups. In Figs 3 ~ 5, the results of the 60 MWd/kgU burnup step were compared for ^{238}U, ^{235}U, and ^{239}Pu which are dominant resonance isotopes in view of number density and the resonance interference effect. The conventional resonance interference method was not compared because its result is almost same with that of the Bondarenko iteration method.

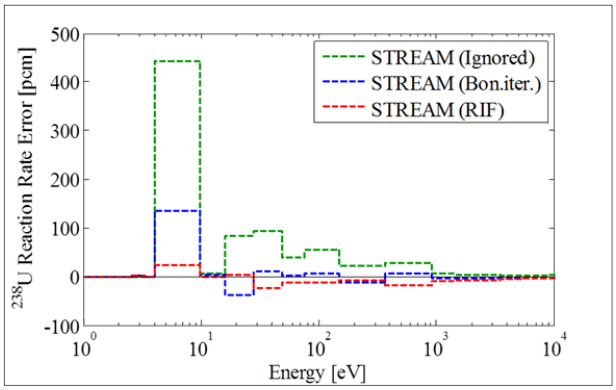

Fig. 3. ^{238}U absorption Reaction rate comparison (Burnup: 60 MWd/kgU)

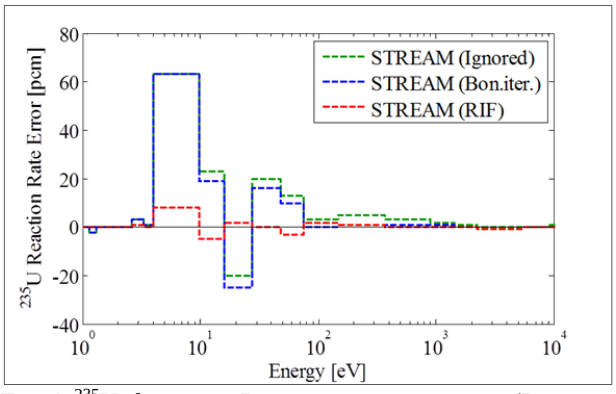

Fig. 4. ^{235}U absorption Reaction rate comparison (Burnup: 60 MWd/kgU)

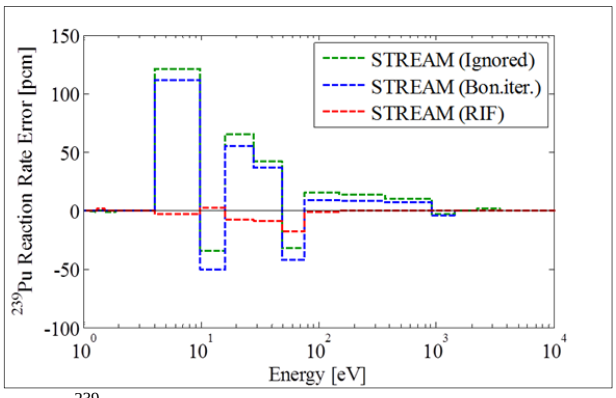

Fig. 5. ^{239}Pu absorption Reaction rate comparison (Burnup: 60 MWd/kgU)

Through Figs 3 to 5, the Bondarenko iteration method shows smaller error than STREAM (ignored) on average, but it cannot handle the resonance interference effects accurately. In some cases, the Bondarenko iteration

method adds more errors than the STREAM (ignored) case.

In Fig. 4, the Bondarenko iteration method does not show improvement in ^{235}U reaction rate between 16.0 eV and 27.7 eV. In the energy group, STREAM (ignored), STREAM (Bon.iter.), and STREAM (RIF) show -20 pcm, -26 pcm, and 2pcm of error in reaction rate, respectively. The Bondarenko iteration method increases the error in the given energy group in contrast to the method using RIF library.

In the conventional and the Bondarenko methods, the background XS of the target isotope increases because of additional absorption XSs from other resonance isotopes. On the other hand, in some cases because of the resonance interference effects, the absorption XSs should be decreased depending on how the resonances overlap each other, and the resonance interference effects can increase or decrease the effective XS of the target isotope. In Fig. 5, this behavior was also observed in ^{239}Pu reaction rates between 9.88 eV and 16.0 eV, and between 48.1 eV and 75.5 eV. The RIF library method shows improvements in predicting the reaction rates compared to STREAM (ignored), while the Bondarenko iteration method adds much error. This behavior will be treated in more detail in section 3.4.

The new RIF library method shows a quite accurate reaction rate compared to the other methods for all isotopes and energy groups in Figs 3, 4, and 5. The maximum error was observed as -27 pcm error of ^{238}U reaction rate between 27.7 eV and 48.1 eV.

3.4 Limitation of the Conventional Methods

In the previous section, the Bondarenko iteration method showed worse results in several energy groups. That is because the conventional resonance interference model and the Bonderenko iteration method simply add absorption XSs of other resonance isotopes into the background XS of the target isotope. These methods can be correct if the absorption XSs of other isotopes are flat within an energy group. However, the resonances have very complicated shapes and those make deep flux distribution. Therefore, the resonance interference effects should be treated by UFG calculation not by MG methods such as the conventional methods. The behavior can be explained clearly by comparisons of ^{150}Sm reaction rates and capture XSs. Similarly with section 3.3, the last burnup step was selected. XS and the reaction rate of ^{150}Sm were compared and shown in Figs. 6 and 7.

In Fig. 6, the Bondarenko iteration method shows larger capture XS in energy between 16.0 eV and 27.7 eV than STREAM (ignored) because of increasing the background XS, but STREAM (ignored) already has a positive XS error. Therefore, the Bondarenko iteration method adds larger error to the XS, and then it increases the error of reaction rate. On the other hand, the new RIF library method predicts the capture XS and the reaction rate accurately. There is -1 pcm of reaction rate error by the RIF method.

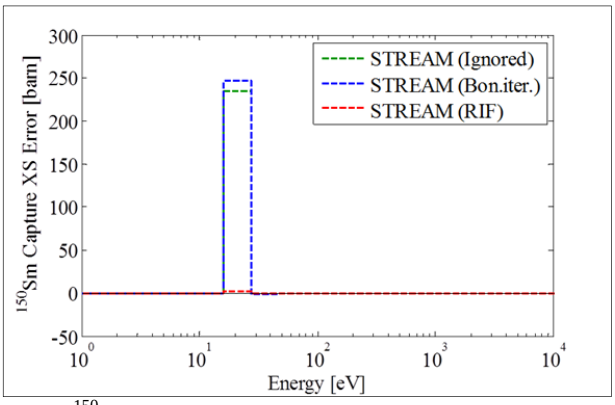

Fig. 6. ^{150}Sm capture cross section comparison (Burnup: 60 MWd/kgU)

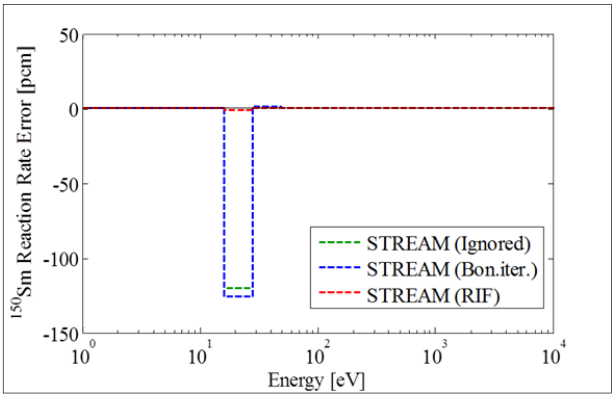

Fig. 7. ^{150}Sm absorption Reaction rate comparison (Burnup: 60 MWd/kgU)

In order to confirm the limitations of the conventional method, UFG group flux spectrums were calculated. As shown in Fig. 8, ^{238}U makes a big dip in the flux between 16.0 eV and 27.7 eV.

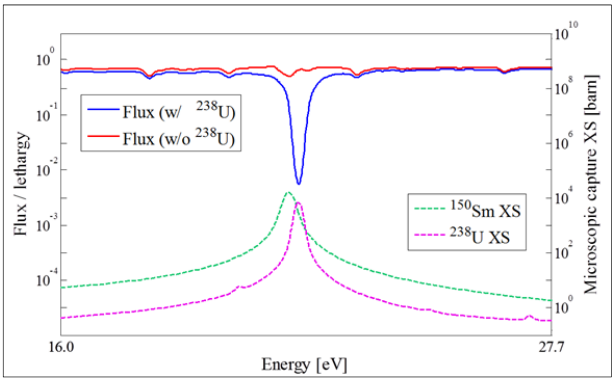

Fig. 8. Ultra-fine-group fluxes and capture cross sections of ^{150}Sm and ^{238}U

The flux dip near 21 eV has a significant impact on the effective XS calculation of ^{150}Sm. The peak of ^{150}Sm resonance is close to 21 eV. If the flux dip is placed near the resonance peak, flux weighting on the resonance peak of resonance is decreased, therefore the effective XS is decreased compared to when the flux dip does not exist. This means that the resonance interference effect does not guarantee increasing the background XS and the effective XS. This behavior should be considered in UFG calculations like the new RIF method, not by MG methods such as the conventional and Bondarenko iteration methods.

4. Conclusions

A new resonance interference model based on the RIF library has been developed and verified. The method interpolates the RIF in the RIF library and uses it to treat the resonance interference effect. The RIF library method has been compared to the conventional resonance interference method and the Bondarenko iteration method. From the verification results, the RIF library method shows less than 73 pcm of error for all burnup steps while the conventional method and the Bondarenko iteration method show 200 ~ 400 pcm of error in early burnup steps. In addition to eigenvalue comparison, detailed reaction rate comparisons were performed. Although the Bondarenko iteration method shows a small error of eigenvalue in the end of burnup step, it has a large error in reaction rates of ^{238}U, ^{235}U, and ^{239}Pu, and much of the error canceled each other. On the other hand, the new RIF method has a maximum -27 pcm of error in ^{238}U reaction rate. The RIF method shows accurate reaction rates for those three isotopes and for all energy groups.

The proposed RIF method is not only accurate but also fast because the method does not require a heavy computation burden such as UFG slowing down calculation during execution. Therefore the RIF method can be used in practical reactor design. Further work will be done to apply the RIF method to general cases.

ACKNOWLEDGMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korean government (MSIP). This work was also partially supported by KETEP, which is funded by the Korean government Ministry of Trade, Industry and Energy. (No. 20131610101850)

REFERENCES

[1] S. Choi, H. Lee and D. Lee, “Status of Deterministic Transport Code Development at UNIST”, *Transactions of the Korean Nuclear Society*, (2013).

[2] R.J.J Stamm’ler, and M. J. Abbate, “Methods of Steady-State Reactor Physics in Nuclear Design,” *London : Academic Press*, Vol. **111** (1983).

[3] R. J. Stamml’er, et al., “HELIOS Methods,” Studsvik Scandpower Internal Report (1998).

[4] D. Knott and A. Yamamoto, "Lattice physics computations." In Handbook of Nuclear Engineering, pp. 913-1239. Springer US, (2010)

[5]. M. L. Williams, “Correction of Multigroup Cross Sections for Resolved Resonance Interference in Mixed Absorbers,” *Nucl. Sci. Eng.*, **83**, 37-49, (1983).

[6]. E. Wehlage, D. Knott and V. W. Mills,” MODELING RESONANCE INTERFERENCE EFFECTS IN THE LATTICE PHYSICS CODE LANCER02,” *M&C*, Palais des Papes, Avignon, France Sep 12-15, (2005).

[7] J. Rhodes, K. Smith, and M. Edenius, "CASMO-4E Extended Capability CASMO-4 User’s Manual," Studsvik Scandpower Report SSP-09/442 –U Rev 0, (2009).