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Application of Resonance Interference Factor generated by Heterogeneous Slowing-down calculation in KARMA

Chae Ho Lim*, Hae Chan Lee and Hae Seuk Woo

*KEPCO Nuclear Fuel Company, #242, Daedeok-daero, 989beon-gil, Yuseong-gu, Daejeon, 34057, Korea,*lcho87@knfc.co.kr*

Abstract - *KARMA code is currently used to nuclear design for the domestic PWRs in KNF (KEPCO Nuclear Fuel Company). The accuracy of the code highly depends on the resonance interference effect treatment. The Bondarenko iteration method was adopted in KARMA to consider the resonance interference effect, but there exist several limitations. In order to reflect the resonance interference effect instead of the Bondarenko iteration, the RIF (Resonance Interference Factor) generated by heterogeneous slowing-down calculation is applied to KARMA. The implementation of the RIF library method is verified for UO_2 and MOX pincell problems, and the verification results show that the code provides more accurate reactivity and reaction rate than the conventional interference method.*

I. INTRODUCTION

KEPCO Nuclear Fuel Company (KNF) has developed the transport lattice code called KARMA (Kernel Analyzer by Ray-tracing Method for fuel Assembly) to be used in the nuclear design for the domestic PWRs. This code adopts MOC (Method Of Characteristics) for the spatial discretization, subgroup method for the resonance treatment and exponential matrix method with Krylov subspace method for the burnup calculation. The multigroup cross section libraries are provided by the KNF library processing system (LICOS)[1].

KARMA adopts the equivalence theory[2] and the Bondarenko iteration method[3] to generate the effective cross sections of resonance energy group. For the resonance treatment method which is based on the equivalence theory, it is important to consider the resonance interference effect among resonance isotopes in estimating the effective cross sections which ultimately lead to the high accuracy prediction on reactivity. However, the subgroup and Bondarenko iteration method have a weakness in estimating the interference effect, which results in non-negligible errors in calculating the effective cross sections. The subgroup parameters used in KARMA are generated at variable temperatures and dilution cases for each single resonance isotope by solving the slowing-down calculation with the ultrafine group cross sections. The interference effect between the resonance isotopes is neglected in this step and is treated at the resonance energy group by using the Bondarenko iteration. But, the treatment of the resonance interference effect cannot deal with the resonance interference occurred within themselves. In the Bondarenko iteration method, the cross sections of other resonance isotopes are constant within a broad energy group. So, exact resonance interference effect cannot be predicted.

In order to reflect the resonance interference effect instead of the Bondarenko iteration, the RIF (Resonance Interference Factor) library method presented by UNIST[4] is applied to KARMA. In this method, the RIF library is pre-generated by the ultrafine group slowing-down calculation. In KARMA code system, the RIFs are generated by heterogeneous slowing-down calculation for a pincell. KARMA code corrects the effective cross section by the interpolated RIF from the RIF library. In this paper, the RIF Library method implemented in KARMA will be verified by its results for UO_2 and MOX pincell problems.

II. RESONANCE INTERFERENCE MODEL IN KARMA

In order to consider the resonance interference effect in KARMA, subgroup method[5] and Bondarenko iteration method are used in the process of calculating the effective cross sections of resonance energy group.

First, KARMA calculates the nuclide number densities by using the information (e.g., material densities, weight fractions of composing nuclides) and atomic masses. Then, slowing down calculations at each subgroup levels are performed to calculate the heterogeneous background cross sections and equivalence cross sections for the reference isotopes of each resonance category. After that, the equivalence cross sections versus the subgroup levels for each isotopes of resonance category are calculated excluding the reference isotopes. Finally, the Bondarenko iteration is performed using the above calculated values to reflect the resonance interference effect and generate the effective cross sections of resonance energy group. Before going to the Bondarenko iteration, the macroscopic background cross section (Σ_{ibn}) for each resonance isotope *i* and subgroup level *n* is calculated. Then, the effective absorption cross section (σ_{ia}) of a resonance energy group is obtained by the Bondarenko iteration to consider the interaction between the resonance nuclides as the following equations:

$$\sigma_{ia} = \frac{1}{N_i} \frac{\sum_n w_{ni} \frac{\Sigma_{ian}\Sigma_{ibn}}{\Sigma_{ian}+\Sigma_{ix}+\Sigma_{ibn}}}{1-\sum_{j=all}\sum_n w_{jn} \frac{\Sigma_{jan}+\Sigma_{jx}}{\Sigma_{jan}+\Sigma_{jx}+\Sigma_{jbn}}}, \qquad (1)$$

where

$$\Sigma_{ibn} = \sum_{j=all} \lambda_j N_j \sigma_{jp} + \Sigma_{ien} , \quad (2)$$

and

$$\Sigma_{ix} = \sum_{j \neq i} N_j \sigma_{ja} . \quad (3)$$

where N_i is the number density for resonance isotope i, Σ_{ian} and Σ_{jan} is the macroscopic absorption cross section for resonance isotope i and j, Σ_{ix} is the sum of macroscopic absorption cross section except resonance isotope i, and ω_n is subgroup weight. Since Σ_{jx} depend on Σ_{ia}, iterations are required. The iteration procedure is as follows:

$$\Sigma_{ix}^{(0)} \rightarrow \Sigma_{iax}^{(0)} \rightarrow \Sigma_{ix}^{(1)} \rightarrow \Sigma_{iax}^{(1)} \rightarrow \Sigma_{ix}^{(2)} \rightarrow \Sigma_{iax}^{(2)} \rightarrow . \quad (4)$$

The denominator of eq. (1) represents the flux, which consider all the flux dips caused by the resonance isotopes individually. But, as described in the above, the subgroup and Bondarenko iteration method have a weak accuracy of treating the interference effect.

III. RIF LIBRARY METHOD IN KARMA

For considering the resonance interference effect, the RIF library method is applied to KARMA. In the RIF method, the effective cross section generated by KARMA is corrected with the corresponding RIF. The RIF for the each resonance isotope i is described in the following equation:

$$RIF_{x,g}^{i \leftarrow j} = \frac{\sigma_{x,g}^{i,mix}}{\sigma_{x,g}^{i,iso}} = \frac{\sum_{u \in g} \sigma_{x,u}^{i} \phi_u^{mix} / \sum_{u \in g} \phi_u^{mix}}{\sum_{u \in g} \sigma_{x,u}^{i} \phi_u^{iso} / \sum_{u \in g} \phi_u^{iso}} \quad (5)$$

ϕ_u^{mix} : Ultrafine group flux for the mixture of all resonance isotopes

ϕ_u^{iso} : Ultrafine group flux for isolated resonance isotope

where x is the reaction type, g is the index of multigroup, and i , j are indices for the resonance isotope.

In the RIF library method presented by UNIST, RIFs are pre-generated by the ultrafine group slowing down calculation for a homogeneous mixture. In case of the KARMA code system, the RIF should be generated by the ultrafine group slowing down calculation for a heterogeneous pincell. The ultrafine group slowing down calculation is performed by EXUS[6] code which was developed by SNU.

In generating the KARMA cross section library, the heterogeneous pincell calculation is performed to obtain an effective resonance cross section from the ultrafine group cross sections. To ensure consistency in generating the RIF library, the RIF is generated by the heterogeneous slowing-down calculation.

Difference of the multigroup resonance absorption cross section for U-238 between the heterogeneous and homogeneous pincell is calculated by the MCNP5, and the results are shown in the Table I. The MCNP5 calculation is performed for the typical UO_2 pincell and the fuel rod is loaded with 5.0 w/o UO_2 fuel. The maximum standard deviation of MCNP5 result is about 10 pcm. Among the 47 group cross section library of KARMA, there are 16 resonance energy groups. Through the MCNP5 calculation for heterogeneous and homogeneous pincell, the 16 group resonance absorption cross sections are generated.

Table I. Difference of multigroup resonance absorption cross section for U-238

Energy group	HET	HOM	Diff (%)
10	1.50E+01	1.55E+01	3.40
11	1.47E+01	1.55E+01	5.79
12	1.75E+01	1.92E+01	9.67
13	1.43E+01	1.52E+01	6.39
14	2.18E+01	2.48E+01	13.60
15	1.44E+01	1.61E+01	12.26
16	8.86E+00	8.86E+00	0.03
17	1.03E+01	1.03E+01	0.11
18	1.48E+01	1.48E+01	0.13
19	8.18E+01	1.01E+02	23.84
20	1.89E+01	1.99E+01	5.22
21	9.64E+00	9.65E+00	0.03
22	9.14E+00	9.14E+00	0.00
23	9.24E+00	9.24E+00	0.00
24	9.22E+00	9.22E+00	0.01
25	9.38E+00	9.38E+00	0.00

As shown in the Table I, the maximum difference of resonance absorption cross section for U-238 is about 24 % between the heterogeneous and homogeneous pincell calculation at near 7.33 eV. Since this difference can make the error in generating the RIF, the RIF library should be generated by the heterogeneous slowing-down calculation in the KARMA code system.

The RIFs are calculated as a function of background cross sections, number density ratios, and temperatures. The RIF library is generated for each resonance isotope, energy group and reaction type. Since the background cross section varies according to the various conditions (e.g., number density of resonance isotope, temperature, spatial effect, etc.), determination of the background cross section grid is especially important in order to generate the accurate RIFs. It is shown in Fig. 1 and 2, which represent the distributions of U-235 and U-238 background cross section for the resonance energy region, respectively. These distributions are calculated from the UO_2 single pincell problem in KARMA. The 'sub' means that subring

of fuel region and lower number denotes that outside of fuel region.

As described in section II, the background cross section (σ_{ibng}) for each resonance isotope *i* and subgroup level *n* is calculated by the slowing down calculations at each subgroup levels. Then, the effective absorption cross section (σ_{iag}) of a resonance energy group is obtained using the corresponding background cross section. However, the background cross section for the RIF library isn't a function of the subgroup level. To calculate the background cross section (σ_{ibg}), the slowing down calculation is performed using the effective cross section generated by the subgroup method. Then, the background cross section is obtained by the following equation:

$$\sigma_{ibg} = \frac{\sigma_{iag}\phi_{ig}}{1-\phi_{ig}} \qquad (6)$$

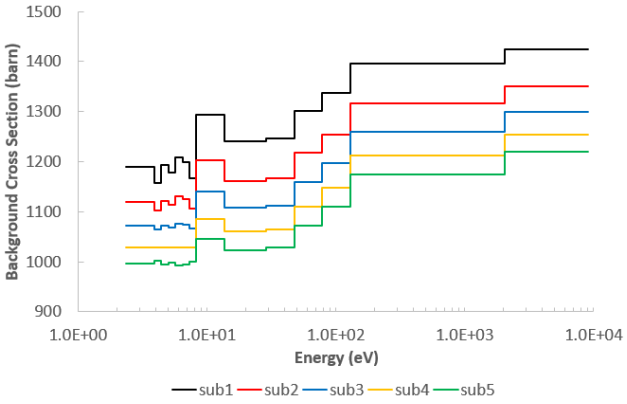

Fig. 1. Distribution of U-235 background cross section.

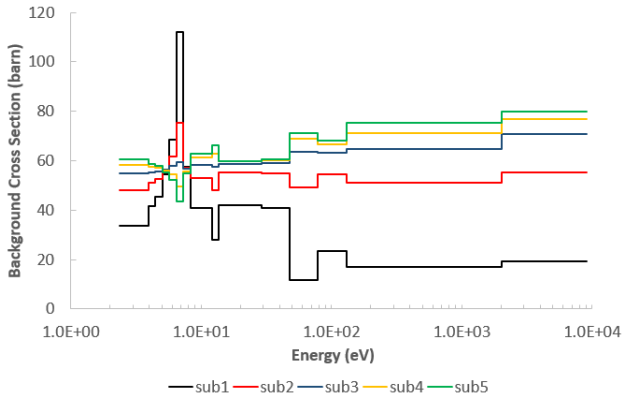

Fig. 2. Distribution of U-238 background cross section.

As shown in the figures, the background cross section is widely distributed depending on the resonance isotope, resonance energy group, and spatial position. The background cross section grid of RIF library should cover possible range of the background cross section for each resonance isotopes.

Since the number of resonance isotopes increases as burnup increases, the RIF library method assumes that interference effect of more than two resonance isotopes is the same as the sum of interference effect between two resonance isotopes. The effective cross section is corrected in KARMA on the assumption by the following equation:

$$\hat{\sigma}^{i}_{x,g} = \sigma^{i}_{x,g} + \sum_{j \in fuel} [\sigma^{i}_{x,g}(RIF^{i \leftarrow j}_{x,g} - 1)] \qquad (7)$$

IV. RESULTS

1. UO_2 pincell problem

The implementation of the RIF library method in KARMA is verified for the UO_2 single pincell problem. The configuration of the single pincell problem is illustrated in Fig. 3. The pincell consisting of UO_2 fuel pellet, Zr cladding and moderator is prepared to simulate the typical 17x17 PWR fuel assembly specification. The fuel rod is loaded with 1.0, 2.0, 3.0, 4.0, and 5.0 w/o UO_2 fuel. The calculations are performed at 1100 K for fuel and 600 K for cladding and moderator. The boundary condition is assumed by reflective boundary condition.

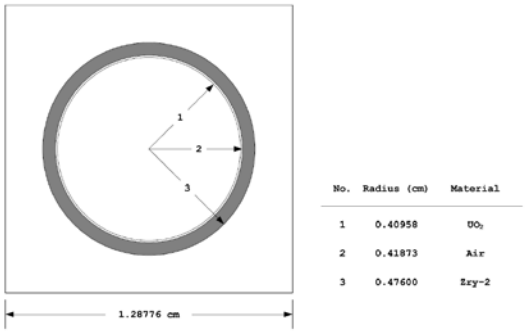

Fig. 3. Configuration of UO_2 single pincell problem.

The reference data is generated by the same KARMA calculation using absorption and fission cross sections generated from MCNP5. The maximum standard deviation of MCNP5 results is about 10 pcm for each problem. Since the interference effect among resonance isotope is perfectly reflected in the cross sections, verification results only show the difference by the interference treatment.

The multiplication factors and absorption reaction rates are calculated for the pincell problem. Fig. 4 shows the difference of the multiplication factor. As shown in the figure, three methods for the resonance interference treatment are compared. The 'RIF' means that the RIF library method, 'Bon.Iter' means that the Bondarenko iteration method, and 'Ignored' means that resonance interference effect is ignored.

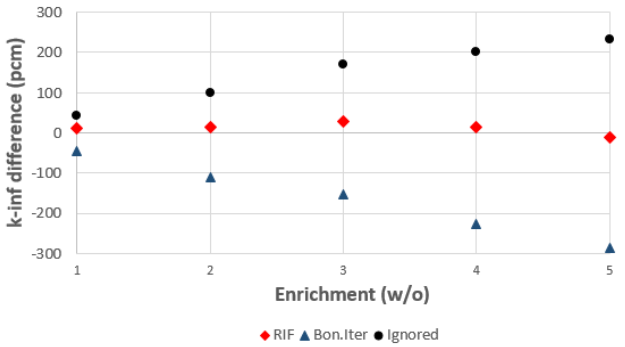

Fig. 4. Difference of the multiplication factor for UO_2 pincell problem.

If the resonance interference effect is ignored, the reactivity is overestimated for all test cases and the maximum error is about 200 pcm for 5 w/o UO_2 pincell case. The difference of the multiplication factor increases as the enrichment increases.

In the Bondarenko iteration method, the background cross section of the target isotope increases because of addition of the absorption cross sections from other resonance isotopes. The Bondarenko iteration method shows larger absorption cross section than that of MCNP5 because of the increasing background cross section. Therefore, the reactivity is underestimated in case of the Bondarenko iteration method compared with the reference calculation as shown in Fig. 4.

The RIF library method predicts the absorption cross section accurately. As the result, the RIF library method provides better multiplication factors compared with the other two methods. The k-inf differences of RIF library method in KARMA are less than 30 pcm for all the UO_2 enrichment cases.

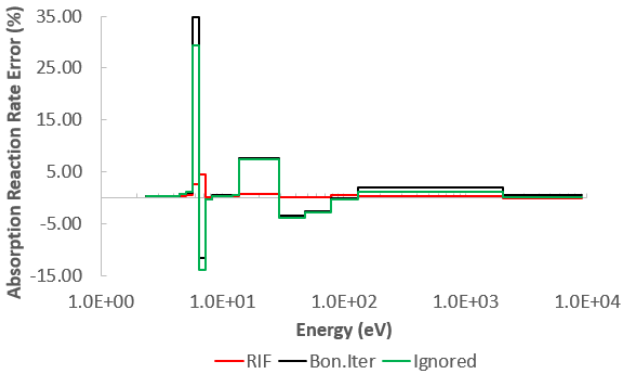

Fig. 5. U-235 Absorption Reaction Rate Error for 5.0 w/o UO_2 fuel.

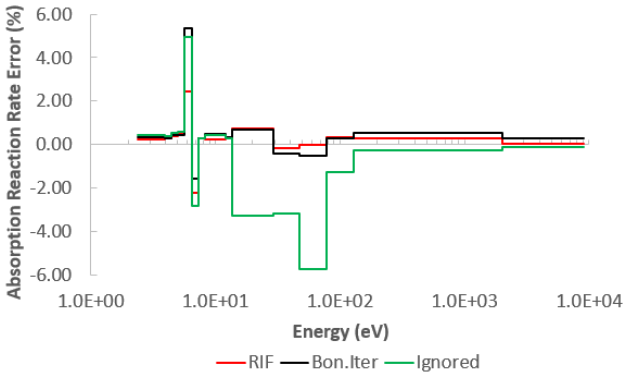

Fig. 6. U-238 Absorption Reaction Rate Error for 5.0 w/o UO_2 fuel.

For detail analyses, absorption reaction rate comparison is performed for U-235 and U-238. The above Figs 5 ~ 6 show the U-235 and U-238 absorption reaction rate error for 5.0 w/o UO_2 pincell case. In Figs 5 ~ 6, the 'Bon.Iter' and 'Ignored' results show larger error than 'RIF' results on average. The RIF library method shows accurate reaction rate compared to the other method. Especially the absorption reaction rate error of U-235 decreases drastically, while the other method shows more than 30% error. Also, the maximum error for U-238 which largely affects the reactivity value decreases in the 'RIF' results. From the above results, the RIF library method shows the improvements in predicting the reaction rates compared to the other methods.

2. MOX pincell problem

In the UO_2 pincell problem, there is only two major resonance isotopes (U-235 and U-238). The resonance interference treatment for fresh UO_2 fuel is simple because only the two isotopes need to be considered. In contrast, the possible fuel compositions are more flexible and complicated. To verify when there are several resonant isotopes in mixture, the MOX pincell problem is prepared. The configuration of the MOX single pincell problem is illustrated in Fig. 7.

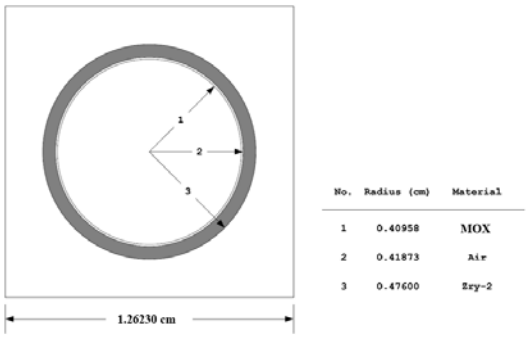

Fig. 7. Configuration of MOX single pincell problem.

The pincell consists of MOX fuel pellet, Zr cladding and moderator. The fuel rod is loaded with 1.0, 2.0, 4.0, 6.0, and 8.0 w/o PuO_2 content for MOX fuel. The calculations are performed at 1100 K for fuel and 600 K for cladding and moderator. The boundary condition is assumed by reflective boundary condition.

The reference data is generated by the same method described in the previous section. For the MOX fuel, cross sections of the Pu isotopes are generated additionally through MCNP5 calculation. The multiplication factors and absorption reaction rates are calculated for the MOX pincell problem as shown in Figs 8 ~11.

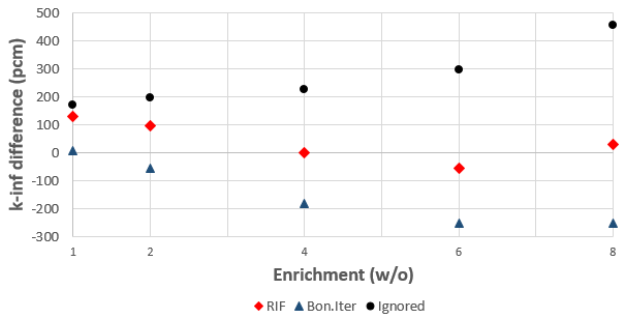

Fig. 8. Difference of the multiplication factor for MOX pincell problem.

If the resonance interference effect is ignored, the reactivity is overestimated for all test cases and the maximum error is about 500 pcm for 5 w/o MOX pincell case. As the number of resonance isotopes increases in the MOX fuel, the difference is larger than the fresh UO_2 fuel.

The Bondarenko iteration method shows smaller reactivity than the reference result like the previous UO_2 pincell problem. This method seems to give accurate results in the low enrichment case (1 and 2 w/o MOX fuel). For this result, a detailed reaction rate comparison is performed to verify whether it is an error cancelation effect or not.

The RIF library method shows less than 100 pcm differences except 1 w/o MOX pincell problem. The maximum difference is 131 pcm for the case.

Figs 9 ~ 11 show U-235, U-238, and Pu-239 absorption reaction rate error for 1.0 w/o MOX fuel. The three isotopes are dominant resonance isotopes in terms of the number density and the resonance interference effect for the MOX pincell problem.

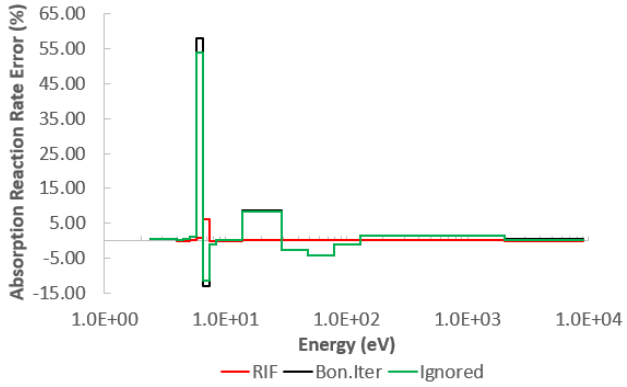

Fig. 9. U-235 Absorption Reaction Rate Error for 1.0 w/o MOX fuel.

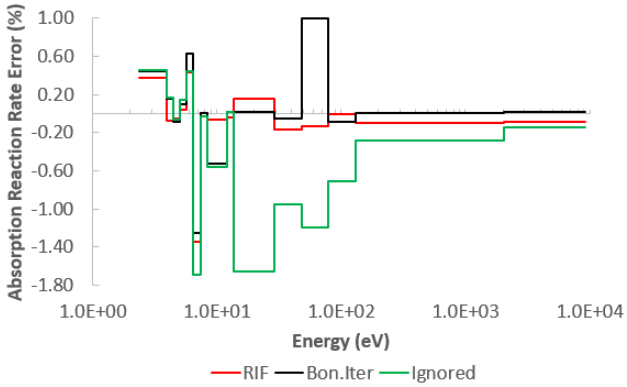

Fig. 10. U-238 Absorption Reaction Rate Error for 1.0 w/o MOX fuel.

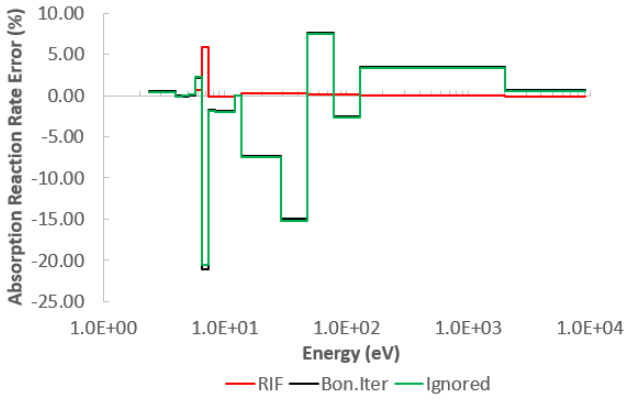

Fig. 11. Pu-239 Absorption Reaction Rate Error for 1.0 w/o MOX fuel.

As shown in the Figs. 9 ~ 11, the absorption reaction rate error of the Bondarenko Iteration method is larger than that of the RIF library method. But the Bondarenko Iteration method shows better results for the 1.0 w/o MOX pincell problem as described in the above. This can be

attributed to the error cancelation among the resonance isotopes when the Pu-239 is added.

Even though the RIF library method shows smaller error than the Bondarenko Iteration method for the 1.0 w/o MOX pincell problem, the reactivity difference is larger than the Bondarenko Iteration method. This error is originated from other cause, but it can be concluded that the RIF library handles the resonance interference effects accurately.

V. CONCLUSIONS

In order to improve the treatment of the resonance interference effect, the RIF library method is applied in KARMA. To generate the RIFs, ultrafine group slowing down calculation is performed for the heterogeneous geometry by EXUS. The RIF values are generated using the equation (5) through the heterogeneous slowing down calculation. Then, KARMA uses the pre-generated RIF library to reflect the interference effect.

The multiplication factors and reaction rates of three kinds of method are compared with the reference results. As shown in the results, the modified KARMA code can provide more accurate multiplication factors for UO_2 and MOX pincell problem compared with the Bondarenko iteration method. In terms of the reaction rate, the RIF library method predicts that accurately while the Bondarenko iteration method shows much larger error.

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