

Heterogeneous Pseudo-Resonant Isotope Method for Resolved Resonance Interference Treatment in Resonance Self-Shielding Calculation

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Abstract — *The theory of resonance interference factor (RIF) method is examined for thermal reactor problems, and the approximations and limitations are identified. To evaluate the interference effect between resonance isotopes, the RIF method establishes an approximate equivalent relationship between a heterogeneous system and a homogeneous system by introducing background cross sections, and the approximation is a source of deviation in self-shielding calculations. Furthermore, each resonance isotope is treated individually in the self-shielding procedure, which requires unnecessary calculation effort, especially for whole-core and burnup cases. Based on the analysis, a heterogeneous pseudo-resonant isotope method (HPRIM) is proposed to overcome these problems. The mixture of resonant nuclides is considered as a pseudo-resonant isotope, and the resonance integral is generated in a one-dimensional heterogeneous system. The numerical results show that HPRIM improves the accuracy of evaluating the resonance interference effect and improves the efficiency of the self-shielding procedure.*

Keywords — *Resonance self-shielding calculation, resonance interference, resonance integral.*

Note — *Some figures may be in color only in the electronic version.*

I. INTRODUCTION

In a recent trend in reactor physics, deterministic neutron transport calculations are directly performed on whole-core problems to achieve high fidelity. Therefore, there will be higher requirements for the accuracy and efficiency of resonance self-shielding treatment.¹ The conventional resonance self-shielding treatment methods for thermal reactor application, including the equivalence theory and subgroup method, require a set of data in the multigroup cross-section library referred to as resonance integral (RI) tables. Generally speaking, RI tables are prepared by performing rigorous ultrafine group (UFG) slowing-down calculations on several homogeneous problems containing one resonant isotope and nonresonant

isotopes with different temperatures and background cross sections.² For equivalence theory,³ RI tables are used for interpolation with the background cross sections of the resonance region in heterogeneous systems to obtain the resonance self-shielded cross sections. In the subgroup method, subgroup parameters are generated from RI tables in the physical probability table approach,^{4,6} except for the mathematical subgroup approach, which does not use RI tables.⁷

RI tables save computational time by prestoring the rigorous results of the self-shielded cross section in each homogeneous problem. However, RI tables are always calculated for only one resonant isotope, and the derivation of both the equivalence and subgroup methods assume just one resonant nuclide in the system. At this stage, the interference effect of different nuclides' resonances is not considered. In fact, neglecting the effect of resonance interference will cause discrepancy when calculating the self-shielded cross

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section, especially in the burnup case. When calculating the self-shielded cross section of some fission products in a burnup fuel, the scalar flux used in weighting the cross section is significantly perturbed by the resonance of ^{238}U , which leads to error in prediction of the number density in burnup calculation. Similar cases happen in mixed-oxide (MOX) fuels because there is also interference between plutonium and ^{238}U .

The information of resonance position and resonance shape of isotopes is lost when pointwise cross sections are collapsed into multigroup cross sections during the slowing-down calculation. In the conventional resonance calculation methods based on RI tables, the resonance interference effect cannot be considered within the process. For the mathematical subgroup approach, subgroup parameters are also prepared for the individual resonant isotope. Various correction treatments and methods were proposed to recover the resonance interference effect after the self-shielding process. Historically, the Bondarenko iteration method has been widely used in lattice physics codes such as CASMO-3 (Ref. 8). The basic idea is considering one resonant isotope in the self-shielding process while the background cross section of each isotope is updated during the iteration to consider the interference effect of other isotopes. Iteration on the background cross section is an efficient way to treat the resonance interference effect because for mixtures of resonant nuclides in a pressurized water reactor (PWR), only a few iterations are required to reach convergence. However, research has shown that there are discrepancies in effective cross-section calculations using iteration procedures, especially in some lower energy groups, where the resolved resonances of different isotopes overlap.^{9,10} During the iteration process, the background cross section of the target resonant isotope is corrected by adding a term described as the average cross section of other isotopes,³ and the iteration process always increases the self-shielded cross section. However, for strong resonance overlap, it has been shown that this overlap underestimates the self-shielded cross section.⁹ The contradiction leads to an overestimation of self-shielded cross section by iteration treatment.

Nowadays, another approach called resonance interference factor⁹ (RIF) has been widely studied to treat the resonance interference effect instead of isotope iteration. The results show that RIF is an effective way to treat the interference effect. However, there are still unknown issues and problems. It is generally acknowledged that RIF is a function of temperature, fuel enrichment, and background cross section. All these parameters are obtained in homogeneous cases, while the actual cases are usually heterogeneous; the validity of RIF in heterogeneous systems has not been fully studied. Another

problem is that RIF requires considerable computational resources from two aspects. One is that RIFs should be carefully calculated and stored, and the second is that the resonance self-shielding procedure should go through every resonant isotope in the mixture to apply RIFs.

In this paper, a thorough investigation of the RIF method is conducted in Sec. II by analyzing the spectra and cross sections of resolved resonance energy groups in several cases. The results show that some inherent discrepancies exist in the RIF method. The error in the resonance self-shielding procedure itself will be brought into the calculation of RIF, and the equivalent relationship between homogeneous and heterogeneous systems used in the RIF method can be a source of discrepancy in some cases. Section III proposes a new method for treating the resonance interference effect by considering the whole mixture of resonant nuclides as a pseudo-resonant isotope and generating the RI tables in heterogeneous systems. Derivations of the theory and calculation flow are given. Theoretically, this new treatment can be coupled with self-shielding methods and reduce the error caused by approximations adopted in the RIF method. Also, a heterogeneous pseudo-resonant isotope method (HPRIM) will significantly reduce the time consumed in resonance self-shielding, thus becoming a promising way to handle large-scale resonance self-shielding problems. In Sec. IV, HPRIM is coupled with an iterative resonance self-shielding method using RI tables,¹⁰ also known as the embedded self-shielding method¹¹ (ESSM). Numerical results show that HPRIM is very effective at obtaining accurate multigroup cross sections considering the resonance interference effect. Section V gives the summary and conclusions.

II. LIMITATIONS OF THE RIF METHOD

II.A. Theory of the RIF Method

During the resonance self-shielding procedure, only one isotope is considered as resonant, and other resonant isotopes are considered as nonresonant. In homogeneous cases with a certain temperature and for a target resonant isotope, the self-shielded cross section is evaluated by background cross section only. The background cross section is defined as

$$\sigma_{b,k} = \frac{\sum_{j \neq k} \lambda_j \sigma_{p,j} N_j + \sum \lambda_m \sigma_{p,m} N_m}{N_k} = \frac{\lambda \Sigma_p - \lambda_k \sigma_{p,k} N_k}{N_k}, \quad (1)$$

where σ_p is the potential scattering cross section and λ is the intermediate resonance (IR) parameter,¹² also known

as Goldstein-Cohen's factor. The subscripts $k, j,$ and m indicate the target resonant isotope, other resonant isotopes that are considered as nonresonant, and moderator, respectively. Potential scattering cross sections of resonant isotopes besides the target are included in the background cross section. Supposing that all the resonant isotopes except the target one are replaced with moderator, and the background cross section remains unchanged, the effective cross section of the target resonant isotope obtained by the self-shielding procedure should remain the same. However, this is clearly not the actual case. Figure 1 shows the fine-structure neutron spectra of the two cases described previously.

Case MIX is a homogeneous mixture containing ^{235}U and ^{238}U as resonant isotopes and H as moderator (mixed condition). Case ISO is a homogeneous mixture containing only ^{235}U as resonant isotopes and H as moderator (isolated condition). The number densities of H and ^{238}U are adjusted so that both cases have the same background cross section for ^{235}U . The spectrum is obtained by rigorous UFG slowing-down calculation. The presence of ^{238}U strongly affects the spectrum of the mixture, and the effective cross section of ^{235}U should be different in the two cases. A comparison of two cases leads to the definition of RIF. The effective cross section is affected by the presence of other resonant isotopes; thus, it can be corrected by a factor that evaluates the difference between the two cases. This factor is defined as

$$f_{x,g}^k = \frac{\sigma_{x,g}^{mix,k}}{\sigma_{x,g}^{iso,k}} = \frac{\int_{\Delta E \in g} \sigma_x^k(E) \varphi^{mix}(E) \Big| \int_{\Delta E \in g} \varphi^{mix}(E)}{\int_{\Delta E \in g} \sigma_x^k(E) \varphi^{iso}(E) \Big| \int_{\Delta E \in g} \varphi^{iso}(E)}, \quad (2)$$

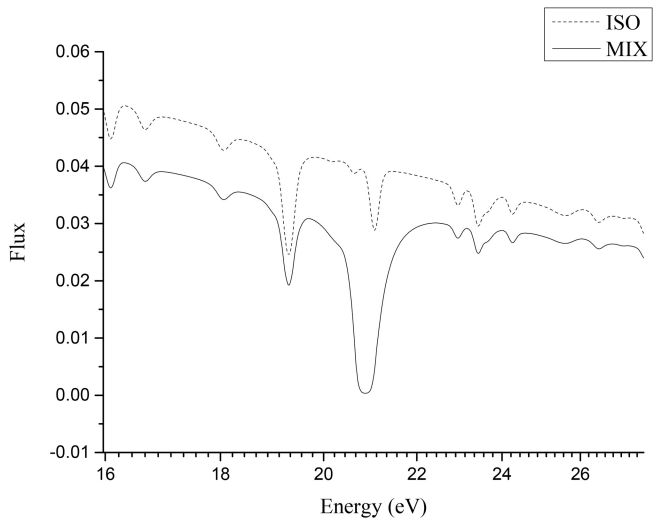


Fig. 1. Comparison of fine-structure neutron spectra between two cases.

where

- $f_{x,g}^k$ = RIF for isotope k , reaction type x , and energy group g
- $\sigma_{x,g}^{mix,k}$ = effective cross section of the MIX case
- $\sigma_{x,g}^{iso,k}$ = effective cross section of the ISO case
- $\sigma_x^k(E)$ = pointwise cross section
- $\varphi^{mix}(E)$ = fine-structure flux of the MIX case
- $\varphi^{iso}(E)$ = fine-structure flux of the ISO case.

RIF is prestored as a function of temperature, background cross section, and ratio of number density or directly calculated instantly. In the conventional resonance self-shielding method, for a target resonant isotope, the effective cross section is first calculated without the interference effect of other resonant isotopes. Then, the effective cross section is multiplied by RIF as a correction taking into account the resonance interference effect.

Decades ago, when the UFG slowing-down calculation was expensive, a rapid approach was proposed to calculate RIF using the analytic form of the spectrum based on the narrow resonance (NR) approximation. The expression of RIF is then rewritten as

$$f_{x,g}^k = \frac{\sigma_{x,g}^{mix,k}}{\sigma_{x,g}^{iso,k}} = \frac{\left\langle \frac{\sigma_x^k}{\Sigma_{a,j} + \lambda \Sigma_{p,j} + \Sigma_{p,m}} \right\rangle_g \left\langle \frac{1}{\Sigma_{a,j} + \lambda \Sigma_{p,j} + \Sigma_{p,m}} \right\rangle_g}{\left\langle \frac{\sigma_x^k}{\sigma_a^k + \sigma_b} \right\rangle_g \left\langle \frac{\sigma_x^k}{\sigma_a^k + \sigma_b} \right\rangle_g}, \quad (3)$$

where

- $\Sigma_{a,j}$ = macroscopic absorption cross section of resonance isotopes mixture
- λ = IR parameter
- Σ_p = macroscopic potential scattering cross section
- σ_b = background cross section of target resonance isotope
- $\langle \rangle_g$ = integration over energy group g .

Another approach is a direct UFG slowing-down calculation on the mixture of resonant nuclides to obtain the rigorous results of fine-structure flux in Eq. (2). The slowing-down equation in a homogeneous system is simplified as

$$\Sigma_i(E)\phi(E) = \sum_k \int_E^{E/\alpha^k} \frac{dE' N_k \sigma_{cs}^k(E') \phi(E')}{(1 - \alpha^k)E'} \quad (4)$$

Fission, upscattering, and inelastic scattering sources are neglected in the method. In this paper, a one-dimensional (1-D) UFG slowing-down calculation code UFOP based on the collision probability method is used to obtain reference fine-structure spectrum.¹³

RIF calculation based on the IR approximation is very fast compared to the UFG method because solving Eq. (4) is time-consuming due to recursion procedures. However, recent studies of the authors^{14,15} pointed out that the shapes of the spectra obtained by IR approximation and the UFG method are different, leading to discrepancy in the effective cross sections, especially for lower energy groups that contain wide and strong resonance. This is quite severe in thermal reactors because the multiplication factor is sensitive to the cross section in lower energy groups.¹⁵ With the development of computational efficiency, more studies^{11,16} use the UFG slowing-down approach.

In a typical light water reactor (LWR) fuel pin, ²³⁸U is the dominant resonant isotope because its number density is large compared to other resonant isotopes. Therefore, the neutron spectrum of the fuel is mainly affected by the resonance of ²³⁸U. In some studies,¹⁷ the resonance interference effect is only considered between ²³⁸U and other resonance nuclides, and RIFs are tabulated as parts of a multigroup library. However, it was also pointed out that the secondary interference effects should be considered in the resonance interference treatment,⁹ especially in MOX fuel with plutonium. Thus, in the calculation of Eq. (2), the entire mixture of resonant nuclides should be involved in the UFG slowing-down calculations. In this case, it is difficult to tabulate RIFs because too many parameters are required to fully address RIFs besides temperatures and background cross sections. Thus, RIFs are evaluated instantly in the resonance self-shielding process, which requires extra computational efforts in the slowing-down calculation.

II.B. RIF in Heterogeneous Systems

From the discussion in Sec. II.A, the conclusion is that in a homogeneous system, the UFG slowing-down calculation of RIF considering the entire mixture is the most rigorous treatment of the interference effect. However, in the actual process of resonance self-shielding treatment in a PWR configuration, the effect of local heterogeneity should be considered. For a given mixture of resonant nuclide, the RIF of the target isotope depends on the temperature and background cross sections of the target isotope in the homogeneous system. According to

equivalence theory, a relationship between homogeneous and heterogeneous systems is established using background cross sections. Thus, the empirical solution to the RIF in heterogeneous cases is to model a zero-dimensional (0-D) homogeneous case with the same background cross section, temperature, and mixture and use it to evaluate the RIF. To do this, the equivalent background cross section is required to set up the homogeneous cases. In the self-shielding method based on equivalence theory, the background cross section of the fuel region can be obtained by the rational approximation of neutron escape probability³ or by fixed-source transport calculation.¹⁸ In the subgroup method, the corresponding background cross section of the fuel region is not produced; however, it can be reproduced by the equivalence cross section obtained at different subgroup levels.¹⁹ Regardless of the resonance self-shielding method used, once the self-shielded cross section is calculated, the background cross section of the target resonant isotope can always be found by inverse interpolation in the RI tables using the self-shielded cross section.

Figure 2 shows the procedure to perform RIF correction after the resonance self-shielding procedure for each resonant isotope.

For a mixture of resonant nuclides in a heterogeneous system, resonance self-shielding is first performed on one resonant isotope, while other resonant isotopes are treated as nonresonant (i.e., no resonance absorption). Self-shielded cross sections are obtained in the isolated condition (ISO), and background cross sections are then obtained by inverse interpolation in the RI table. A new mixture of resonant nuclides in a homogeneous system is modeled that contains the same number density for each resonant isotope as in the initial case. The new case

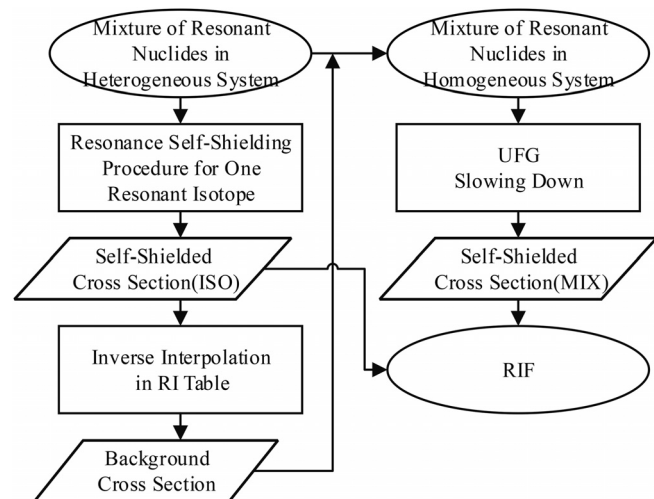


Fig. 2. Procedure of RIF correction for a mixture of resonant nuclides in a heterogeneous system.

maintains the same background cross section of the target isotope by adjusting the number density of moderator isotopes. UFG calculation is performed on the new case, and all resonant isotopes are considered. The self-shielded cross sections of the target isotope considering the interference effect of the mixture (MIX) are obtained. RIF is finally obtained by Eq. (2).

Though the details are different, various methods for treating the resonance interference effect using RIF follow the same procedure. It is also an independent procedure that does not depend on the resonance self-shielding method used. Similar to equivalence theory, this procedure tries to establish an equivalent relationship of the RIF in heterogeneous and homogeneous systems by evaluating the background cross section. However, there are two sources of error involved in the procedure that should be discussed.

The first source of error is the evaluation of the background cross section. Suppose that the RI tables are so detailed that there is no error introduced in the inverse interpolation; still, the groupwise self-shielded cross sections obtained in the isolated condition by different resonance self-shielding methods are not always accurate.

Figure 3 shows the groupwise microscopic absorption cross section errors of a typical LWR fuel pin cell containing only ²³⁸U. Four resonance self-shielding methods are tested:

1. Stamm'ler method of two-term rational approximation with Dancoff factor³
2. generalized Stamm'ler method, used in code DRAGON version 4, SHI: module with Livolant and Jeanpierre normalization scheme²⁰

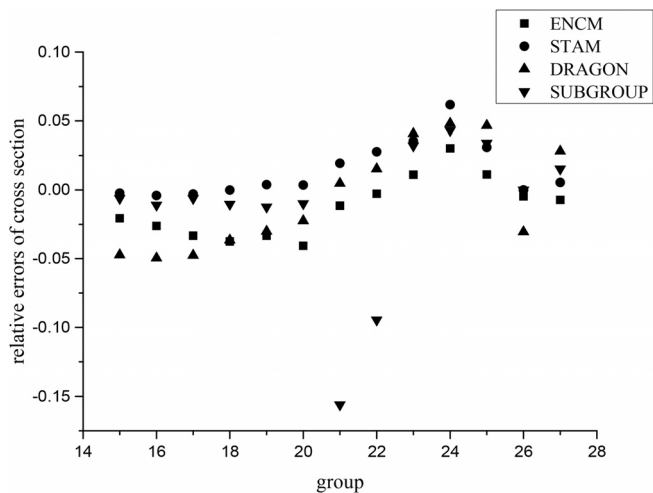


Fig. 3. Relative errors of microscopic absorption cross section obtained by different methods.

3. enhanced neutron current method (ENCM) coupled with AutoMoc code as fixed-source transport solver¹⁸
4. subgroup method used in code SUGAR (Ref. 4).

The WIMS 69-group structure²¹ is adopted, and reference results are obtained by UFOP. The results show that different resonance self-shielding methods cause different levels of error in the microscopic absorption cross section of ²³⁸U. The inherent error in multigroup resonance self-shielding methods when treating heterogeneous cases with one resonant isotope is common because many approximations are involved in these methods. In the authors' previous research,^{14,15} the inherent error in equivalence theory was discussed. For the subgroup method, the NR approximation and the numerical procedure used to generate subgroup levels and weights can also result in discrepancies.

According to the previous discussion, RIF is a function of background cross section and decreases with increasing background cross section. In some energy groups with strong resonance overlap, RIF can be sensitive to the background cross section. In the RI table, background cross section is a function of self-shielded cross section from the aspect of inverse interpolation, and it can also be sensitive in some energy groups with strong resonance. Therefore, RIF is a function of self-shielded cross section obtained in isolated conditions, and the error in the self-shielded cross section in isolated conditions will be brought into the RIF calculation. For example, for a mixture of resonant nuclides with 30 wt% ²³⁵U enrichment, the RIF of ²³⁸U for group 23 (48 to 75.5 eV) is shown in Fig. 4 as a function of the self-shielded cross

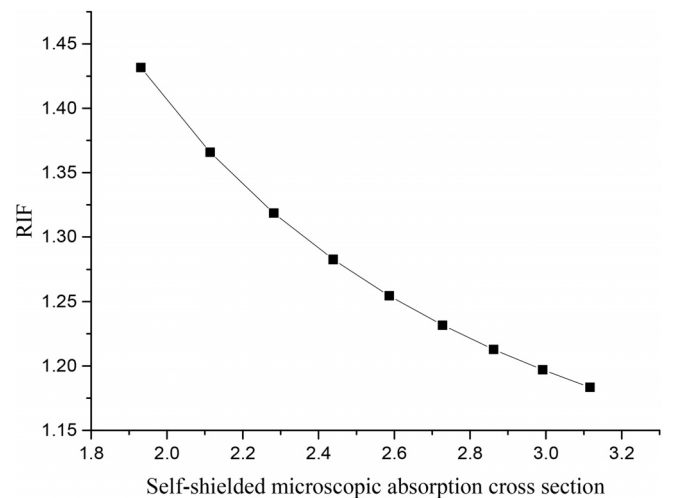


Fig. 4. RIF for different background cross sections and corresponding self-shielded microscopic absorption cross sections in isolated conditions.

section in isolated conditions. This shows that an error of 10% in the self-shielded cross section can cause an error of 4% in the RIF. Therefore, the inherent error in the resonance self-shielding method will be an error source in the evaluation of RIF.

The second source of error is more severe because the equivalence relationship of the RIF between heterogeneous and homogeneous systems is an inherent approximation in the RIF method. The equivalence relationship is used empirically without validation. To narrow down this source of error in the multigroup resonance self-shielding procedure, the UFG slowing-down calculation can be used for “Resonance Self-Shielding Procedure for One Resonant Isotope” in Fig. 2. In other words, in the self-shielding procedure considering only one resonant isotope, the pointwise cross sections of the target resonant isotope is used in the UFG calculation, while other resonant isotopes are considered as moderators with constant potential scattering cross sections. In this way, the first error source is excluded, and the second error source can be evaluated by directly comparing the self-shielded cross sections between the two cases. One is the initial case (mixture of resonant nuclides in a heterogeneous system), and the second is the equivalent case (mixture of resonant nuclides in a homogeneous system). Both of them are calculated by the UFG method considering all resonant isotopes. For a better understanding, the updated procedure is shown in Fig. 5.

Table I shows the second source of error in a fuel pin cell of UO₂ with two different enrichments of ²³⁵U. Groups 23, 24, 25, and 27 are investigated because of the strong resonance of ²³⁸U in these groups.

TABLE I

Percentage Difference for the Two Calculation Procedures

Group	²³⁸ U RIF		²³⁵ U RIF	
	L ^a	H ^b	L	H
23	0.1957%	5.6497%	-0.3373%	-0.1615%
24	0.5158%	4.1789%	-0.0749%	0.4053%
25	0.7294%	5.2368%	0.2211%	0.3699%
27	0.5255%	4.6596%	1.1903%	1.4188%

^aLow-enrichment case composed of ²³⁸U = 0.02, ²³⁵U = 0.001 (10²⁴ atoms/cm³).

^bHigh-enrichment case composed of ²³⁸U = 0.02, ²³⁵U = 0.02 (10²⁴ atoms/cm³).

For the lower-enrichment case, the errors in the original RIF procedures are <1%. However, for the higher-enrichment case, the error in the original RIF procedure increases, especially for ²³⁸U. The higher-enrichment case is an extreme situation that is not common in LWR design. The purpose of this test is to show the theoretical limitations of the RIF method. For MOX fuel and high burnup conditions, the investigation of the RIF method is more realistic.

Table II shows the second source of error in MOX cases with two different enrichments of plutonium.

In this case, the resonance interference effect is more complex than in the previous case, because it contains many resonant isotopes and many resonances that overlap. Similar results can be found for higher enrichments of plutonium, and the RIF procedure’s errors are larger.

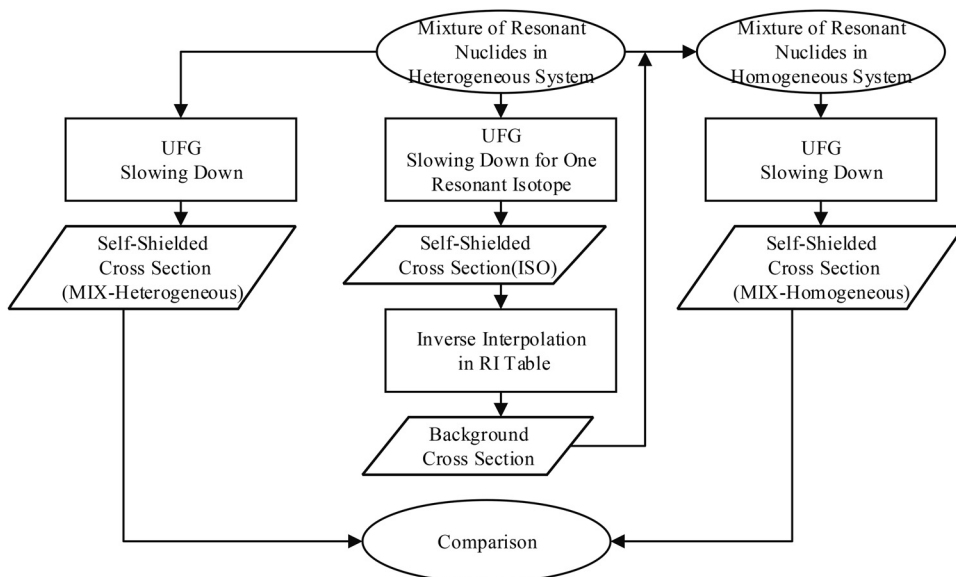


Fig. 5. Procedure of error source evaluation for equivalence relationship of RIF between heterogeneous and homogeneous systems.

TABLE II
Percentage Difference for the Two Calculation Procedures for MOX Pin Cell

Group	²³⁸ U RIF	
	L ^a	H ^b
23	2.4601%	4.5740%
24	1.2360%	1.9208%
25	1.6455%	2.6402%
27	1.7625%	3.0558%

^aLow-enrichment case composed of ²³⁸U = 0.02, ²³⁵U = 0.001, ²³⁹Pu = 0.001, ²⁴⁰Pu = 0.0005, ²⁴¹Pu = 0.0002, ²⁴²Pu = 0.0002 (10²⁴ atoms/cm³).

^bHigh-enrichment case composed of ²³⁸U = 0.017, ²³⁵U = 0.001, ²³⁹Pu = 0.003, ²⁴⁰Pu = 0.002, ²⁴¹Pu = 0.0005, ²⁴²Pu = 0.0004 (10²⁴ atoms/cm³).

The primary cause of the discrepancy in the RIF procedure in Fig. 5 is related to the neutron spectrum used in weighting the cross section. In Fig. 5, the connection between the mixture of resonant nuclides in a heterogeneous system and in a homogeneous system is the background cross section of the target resonant isotope in isolated conditions. As a matter of fact, since the neutron spectra in both systems satisfy the following equation:

$$\int_{\Delta E \in g} \sigma_x^k(E) \varphi_{heter}^{iso}(E) \Bigg| \int_{\Delta E \in g} \varphi_{heter}^{iso}(E) = \int_{\Delta E \in g} \sigma_x^k(E) \varphi_{homo}^{iso}(E) \Bigg| \int_{\Delta E \in g} \varphi_{homo}^{iso}(E) \quad (5)$$

When considering the interference effect from other isotopes, the spectra will be changed to $\varphi_{heter}^{mix}(E)$ and $\varphi_{homo}^{mix}(E)$. Therefore, Eq. (5) will be updated as

$$\int_{\Delta E \in g} \sigma_x^k(E) \varphi_{heter}^{mix}(E) \Bigg| \int_{\Delta E \in g} \varphi_{heter}^{mix}(E) = \int_{\Delta E \in g} \sigma_x^k(E) \varphi_{homo}^{mix}(E) \Bigg| \int_{\Delta E \in g} \varphi_{homo}^{mix}(E) \quad (6)$$

However, Eq. (6) is not strictly true due to two reasons. One is that the original spectra have been perturbed by the resonances of other resonant isotopes. Another one is that the neutron spectrum in a heterogeneous system is different from that in a homogeneous system. Figure 6 compares the spectra of group 25 for heterogeneous and homogeneous systems.

Two cases are tested (low enrichment and high enrichment), and they are the same as in Table I. The spectra are normalized so that the flux integral within the

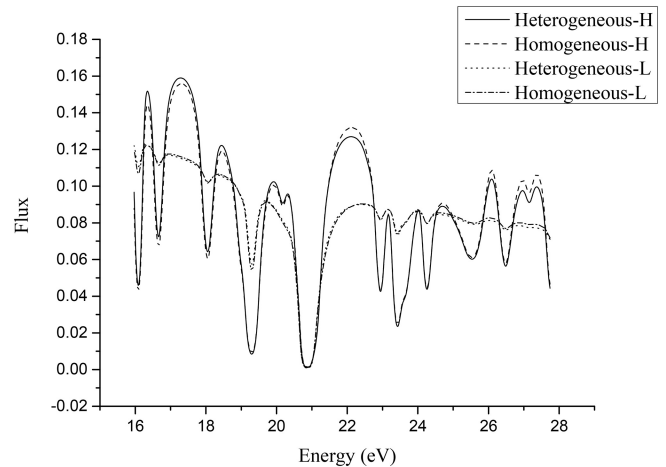


Fig. 6. Spectral comparison between heterogeneous and homogeneous systems within group 25.

group is 1. It is shown that the difference in the spectra of the heterogeneous and homogeneous systems is larger in the high-enrichment case than in the low-enrichment case. The difference between the left and right terms in Eq. (6) is unpredictable because it is affected not only by the level of interference but also by the strength of the resonance. However, the general trend is that the discrepancy is larger for higher-enrichment cases.

To sum up, the discrepancy in the RIF method in heterogeneous systems is thoroughly investigated. One error source is that the multigroup resonance self-shielding method may cause discrepancy in the groupwise self-shielded cross section in isolated conditions due to different adopted approximations, and this discrepancy will be brought into the RIF evaluation. Another error source is that it is not strictly valid to use the background cross section of the target resonant isotope to establish the equivalence relationship between heterogeneous and homogeneous systems. These two error sources are inherent characteristics of the RIF method. The physical explanations of these two issues are listed as follows:

1. The RIF method is still an external correction on the conventional self-shielding calculation frame, which is based on the assumption that there is only one resonant nuclide considered. As a key parameter to obtain the RIF, the background cross section is decided by the self-shielded cross section in isolated conditions, which is sufficiently accurate. Thus, the evaluation of the resonance interference effect is influenced by complex issues.

2. A recent study by the authors¹⁵ pointed out that in the low-energy range (4 to 100 eV), the difference in the shapes of the spectra of homogeneous and heterogeneous systems is large, and the equivalent relationship may fail at a certain resonance. This conclusion also applies to

the equivalent relationship of the resonance interference effect between homogeneous and heterogeneous systems. The difference between the spectra becomes larger when the fuel enrichment increases.

III. HETEROGENEOUS PSEUDO-RESONANT ISOTOPE METHOD

III.A. Theory of HPRIM

In this study, a new method is proposed to fully address resonance interference effects. In this method, the entire mixture of resonant nuclides is considered as a pseudo-resonant isotope, and the RI of the pseudo-resonant isotope is prepared in heterogeneous cases.

In the Stamm'ler method,³ when treating the resonance interference effect by the iteration procedure, the flux is expressed as

$$\phi_m(E) = \frac{\lambda \Sigma_p + \Sigma_{em}}{\Sigma_a(E) + \lambda \Sigma_s + \Sigma_{em}}, \quad (7)$$

where $\Sigma_a(E)$ is the macroscopic absorption cross section of the entire mixture of resonant nuclides. Because there are only RI tables for isolated resonant nuclides in the multigroup library, in the following derivation, the macroscopic absorption cross section is defined as

$$\Sigma_a(E) = \Sigma_{a,k}(E) + \sum_{j \neq k} \Sigma_{a,j}. \quad (8)$$

Thus, the iteration among resonant nuclides becomes available.

For Eq. (7), both the numerator and the denominator are divided by the number density of all resonant nuclides, giving

$$\begin{aligned} \phi_m(E) &= \frac{\lambda \Sigma_p / N_{sum} + \Sigma_{em} / N_{sum}}{\Sigma_a(E) / N_{sum} + \lambda \Sigma_s / N_{sum} + \Sigma_{em} / N_{sum}} \\ &= \frac{\bar{\sigma}_{p,r} + \sigma_0}{\bar{\sigma}_{t,r}(E) + \sigma_0}, \end{aligned} \quad (9)$$

where $\bar{\sigma}_{p,r}$ and $\bar{\sigma}_{t,r}(E)$ are the average microscopic cross sections of the entire mixture of resonant nuclides weighted by the number density of each resonant nuclide. Figure 7 shows the average microscopic cross section of a mixture of ²³⁸U and ²³⁵U (5% enrichment of ²³⁵U).

From the aspect of the pointwise cross section, any mixture of resonant nuclides can be treated as a pseudo-resonant isotope with all the weighted resonance. In homogeneous cases, based on the NR approximation, the flux expression can be directly evaluated by Eq. (9) using

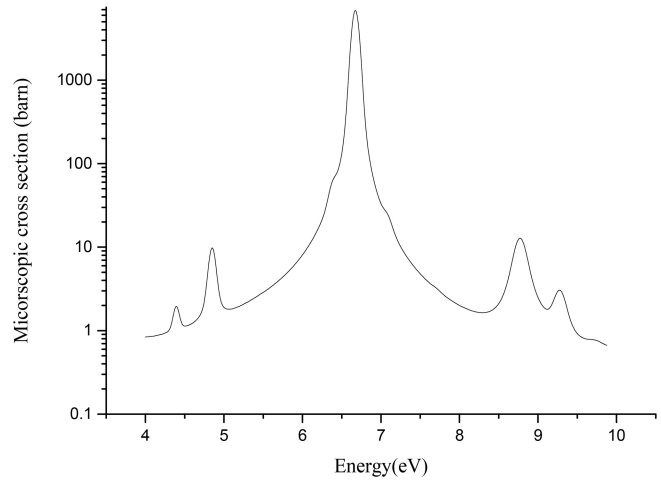


Fig. 7. Average cross section of the mixture of resonant nuclides.

the weighted pointwise cross section of the pseudo isotope. It is well-known that the UFG slowing-down calculation is a more rigorous approach to solving flux; thus, the flux of homogeneous cases with the pseudo-resonant isotope can also be solved by the UFG method. Thus, the multigroup self-shielded cross sections of the pseudo isotope are obtained.

The groupwise self-shielded cross sections of the pseudo isotope can also be defined in an alternative way:

$$\sigma_{x,g}^{pseudo} = \frac{\sum_k N_k \sigma_{x,g}^{mix,k}}{\sum_k N_k}. \quad (10)$$

In Eq. (10), $\sigma_{x,g}^{mix,k}$ in the numerator has the same meaning as in Eq. (2), which is the self-shielded cross section of an isotope considering all the resonance interference in the mixture. The background cross section of the pseudo isotope is redefined as

$$\sigma_{b,pseudo} = \frac{\sum_m \lambda_m \sigma_{p,m} N_m}{\sum_k N_k}. \quad (11)$$

For a certain mixture of resonant nuclides, with UFG slowing-down calculation of homogeneous cases with different temperatures and background cross sections, the RI tables of the corresponding pseudo isotope can be established.

At this stage, the RI tables of pseudo-resonant isotope are constructed and can be directly used by resonance self-shielding methods such as equivalence theory and the subgroup method. As previously stated, equivalence theory and the subgroup method are processed

based on the assumption that there is only one resonant isotope in the system. In this case, the assumption will not bring any discrepancy because there is actually only one resonant isotope, the pseudo isotope.

The pseudo-resonant isotope treatment can be explained in an alternative way. The conventional resonance interference treatments, including the iteration method and the RIF method, focus on the correction of the error brought about by the isolated resonant nuclide assumption, which is a belated effort. However, the concept of pseudo-resonant isotope brings the resonance interference effect into the multigroup library, which is superior to conventional treatments because it is independent of resonance self-shielding methods, and resonance interference evaluation is not influenced by the isolated resonant nuclide assumption.

According to the discussion in [Sec. II.B](#), the treatment of the pseudo-resonant isotope still suffers from the inconsistency between the spectra of the heterogeneous and homogeneous systems in the low-energy range. In some studies,^{10,19} a 1-D heterogeneous problem is used instead of a 0-D homogeneous problem to generate the RI tables. A similar technique can be used for the treatment of the pseudo-resonant isotope. The UFG calculation to determine the self-shielded cross section of the pseudo-resonant isotope is performed for a 1-D heterogeneous problem. For a LWR case, the 1-D heterogeneous problem is a simple two-region pin cell with the pseudo-resonant isotope in the fuel region and H in the moderator region. To prepare the RI table, several 1-D heterogeneous problems with different moderator-to-fuel ratios are calculated. In addition to the self-shielded cross section, the corresponding background cross section of the pseudo isotope is determined differently depending on the resonance self-shielding method used. A few examples are listed as follows:

1. For the Stamm'ler method, rational approximation and Dancoff factor are calculated for the 1-D heterogeneous problem to obtain the background cross section.

2. For ENCM, the background cross section is calculated based on the reaction rate in lattice geometry¹⁸:

$$R_{tot} = \sum_{i,f}(E) \frac{\sum_{s,f} + \sum_e}{\sum_{i,f}(E) + \sum_e} \frac{1}{E} \approx \sum_{s,f} + \sum_e \quad (12)$$

and

$$\sigma_{b,pseudo} = \frac{R_{tot}}{N_{pseudo}} - \sigma_{p,pseudo} \quad (13)$$

In [Eq. \(12\)](#), a very large $\sum_{i,f}(E)$ is assumed, and E is set to unity since E can be chosen arbitrarily.¹⁸

3. For the subgroup method and ESSM, the background cross section is obtained by the method given in [Ref. 19](#):

$$\sigma_{b,g}^{pseudo} = \frac{1}{N_{pseudo}} \frac{\sum_{a,g}^{pseudo} \phi_{f,g}}{1 - \phi_{f,g}} \quad (14)$$

The reaction rate and flux above are obtained by a one-group fixed-source transport calculation over the 1-D heterogeneous problem,

$$\Omega \cdot \nabla \psi_g(\vec{r}) + (\Sigma_{a,g} + \lambda \Sigma_{p,g}) \psi_g(\vec{r}) = \lambda \Sigma_{p,g} \quad (15)$$

In [Eqs. \(14\)](#) and [\(15\)](#), $\phi_{f,g}$ is the scalar flux integrated by $\psi_g(\vec{r})$.

In these examples, all the resonant isotopes are considered together as a pseudo-resonant isotope, and the number densities used are the same as in [Eq. \(10\)](#). After the corresponding background cross sections are obtained, the RI tables of the pseudo-resonant isotope are established. Meanwhile, during the UFG calculation, the RI tables of each resonant isotope with interference effect are also prepared, and the corresponding background cross section is defined as in the RI tables of the pseudo isotope instead of as in [Eq. \(1\)](#).

Going back to the procedure in [Fig. 2](#), it is found that the definition of HPRIM could directly retrieve the results of the mixture of resonant nuclides in a heterogeneous system instead of in a homogeneous system, as in the RIF method. Since the multigroup resonance self-shielding method can treat only one resonant isotope at a time for a certain mixture of resonant nuclides (i.e., one pseudo-resonant isotope), resonance self-shielding is performed only one time. For methods based on equivalence theory, the equivalence cross section is obtained by the rational approximation of escape probabilities or fixed-source transport calculation, and the background cross section is then obtained and used to interpolate the RI tables of pseudo-resonant isotopes. For the subgroup method, subgroup levels and weights are obtained by the numerical fitting of RI tables of the pseudo-resonant isotope, and fixed-source transport calculation is performed to calculate the flux in the subgroup, which is used to weight the self-shielded cross section. Theoretically, at this step, it is sufficient to provide the macroscopic resonance self-shielded cross section of the mixture of resonant nuclides and continue the transport calculation. However, the self-shielded cross section of each resonant isotope is also needed because they are essential in burnup calculation. Therefore, for both equivalence theory and the subgroup method, the inverse interpolation on the self-shielded cross section of the pseudo-resonant isotope is necessary

to retrieve the background cross section. Because the RI tables of each resonant isotope with interference effect have been established previously, the background cross section is used for interpolation to obtain the self-shielded cross section of each resonant isotope. The entire procedure is shown in Fig. 8.

HPRIM totally changes the original framework of resonance interference treatment because the resonance interference effect is contained throughout the entire procedure. The main advantage is that HPRIM achieves high accuracy in evaluating the interference effect because it manages to avoid the isolated resonant isotope assumption and also considers the consistency between the spectra of the heterogeneous cases and RI tables. In addition, HPRIM has strong universality for any type of multigroup resonance self-shielding method. In addition, the computational effort for the resonance self-shielding procedure is reduced due to the new framework. Nowadays, to consider the local heterogeneous effect in assemblies or even the whole core, fixed-source transport calculation is usually adopted in the resonance self-shielding procedure, such as ESSM and the subgroup method. The computational effort is concentrated on the fixed-source transport calculation when dealing with a large-scale problem. In the resonant isotope iteration and RIF methods, the fixed-source transport calculation has to go through each resonant isotope in the mixture because the self-shielding procedure has to be performed under isolated conditions. However, these calculations are unnecessary because the local heterogeneous effect depends on the macroscopic cross section of each region. HPRIM considers the whole mixture of resonant nuclides as a pseudo isotope; thus, the

self-shielding procedure is only needed once, saving a large amount of computational effort.

III.B. HPRIM Coupled with ESSM

ESSM is proposed to simplify the subgroup method because it does not need to generate the subgroup parameters and directly use the RI table. From another perspective, ESSM is also based on equivalence theory because the self-shielding procedure is performed to obtain the background cross section of a fuel region considering its local heterogeneous effect. The original ESSM adopted the technique in HELIOS that divides the resonant isotope into categories. ESSM is then updated to use modified RI tables to consider the resonance interference effect. The RI of each resonant isotope is modified by adding a perturbation term for interference between two resonant isotopes. A similar approach is proposed in ESSM (Ref. 11). Theoretically, HPRIM can be coupled with any multigroup self-shielding method; however, ESSM is chosen to test HPRIM instead of the Stamm'ler or subgroup method for the following reasons:

1. Compared to the Stamm'ler method, ESSM can treat irregular geometries by using the MOC transport solver with a better evaluation of the local heterogeneous effect.

2. There are difficulties in generating the subgroup parameters for pseudo-resonant isotopes. Usually, the subgroup parameters are generated with numerical optimization and prestored in the external library. However, for the pseudo-resonant isotope, the subgroup parameters must be generated instantly. The robustness and efficiency of this procedure are still problems for the subgroup method.

A simple description of ESSM is as follows:

1. For each resonant isotope in each region, the effective cross sections at infinite dilution are used as the initial values.

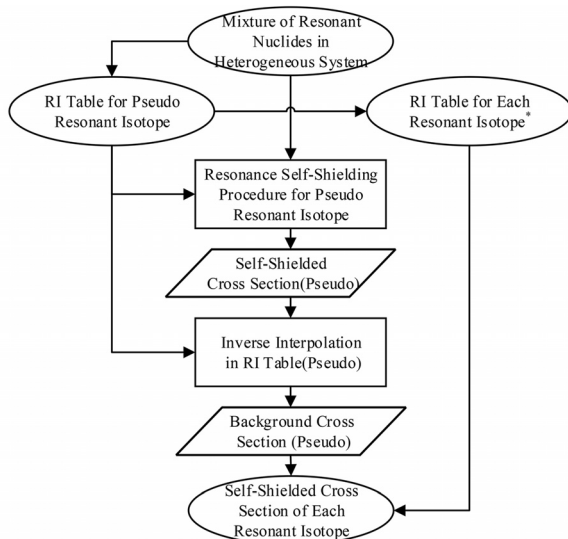
2. Equation (15) is used to perform a one-group, fixed-source transport calculation.

3. The scalar flux obtained in the fuel region is used to calculate the background cross section using Eq. (14).

4. The background cross section is used to interpolate the RI tables to obtain the new effective cross section.

5. Equation (15) is updated, and the procedure starts over at the second step and is repeated until convergence is achieved.

Compared to original ESSM, no consideration of multiple resonant isotopes is needed because there is only



*Contains resonance interference effect

Fig. 8. Calculation procedure of HPRIM.

one pseudo-resonant isotope. The entire calculation flow of HPRIM coupled with ESSM mainly follows the procedure in Fig. 8. The only difference is that no inverse interpolation is needed because the background cross sections are already decided during the previous step.

III.C. Resonance Integral Tables of the Pseudo Isotope

As previously discussed, the pseudo isotope corresponds to the mixture of resonant nuclides. In a practical lattice physics calculation, a number of different mixtures of resonant nuclides are treated with the resonance self-shielding procedure. The most rigorous approach is that for a mixture of resonant nuclides, the pseudo-resonant isotope is constructed, and RI tables are generated instantly. However, in burnup cases, the mixture of resonant nuclides in each fuel region contains many resonance isotopes, and the total number of pseudo-resonant isotopes in each burnup step is large. It is impossible to prestore all the RI tables of pseudo-resonant isotopes because the composition of the fuel is obtained by burnup calculation. Therefore, the UFG slowing-down calculation for 1-D heterogeneous problems will occupy too much time of the lattice physics calculation.

Another approach is proposed to improve the efficiency by setting up multidimensional RI tables for interpolation. For constant temperature and background cross section, the resonance interference effect varies monotonically with the number density of another isotope. A mixture of resonant nuclides of ^{238}U , ^{235}U , and ^{239}U is investigated with different number density ratios. Figure 9

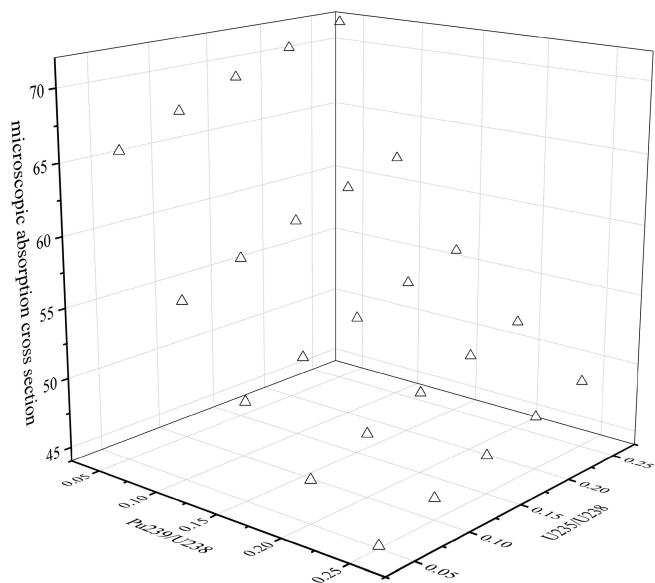


Fig. 9. Microscopic absorption cross section of a mixture of ^{235}U , ^{238}U , and ^{239}Pu

shows the microscopic absorption cross section of ^{239}Pu in group 25 as a part of a pseudo-resonant isotope's cross section.

The results are obtained by the UFG method in cases with different number density ratios and the same temperature and background cross section. Figure 9 shows that the microscopic cross section of each resonant isotope can be tabulated as a function of the number density ratio as

$$\sigma = f(T, \sigma_b, D_{^{235}\text{U}/^{238}\text{U}}, D_{^{239}\text{Pu}/^{238}\text{U}}, \dots), \quad (16)$$

where

T = temperature

σ_b = background cross section

D = number density ratio of each resonant isotope.

Within a limited range of number density ratio of each resonant nuclide, the function shown in Eq. (16) is nearly linear. If a sufficient number of cases with different temperature points, background cross section points, and number density ratio points are calculated, the RI tables of any pseudo-resonant isotope (within the limited range mentioned above) can be calculated by an interpolation procedure.

However, considering all the resonance isotopes for the burnup case within a wide range of number density ratios, variation is unpractical. In the benchmark problem study of LWRs (Ref. 22), 29 resonant isotopes are included in the burnup calculation. RI tables that fully address the interference effect will require millions of UFG calculations. Four measures are taken to reduce the size of the multidimensional RI table:

1. The geometry and moderator composition of the 1-D fuel cell should be close to the target lattice configuration. Only the moderator/fuel ratio changes to obtain different background cross sections.

2. Mixtures of resonant nuclides with similar compositions use the corresponding RI table, especially those fuel regions with the same fuel type.

3. In the benchmark problem study of LWRs (Ref. 22), from 0 to 70 GWd/tonne, variations in the number density of most resonant nuclides are within a limited range. Only two or three number density ratio points are taken for each resonant nuclide.

4. Resonant isotopes are divided into three categories. The first category contains the resonant nuclides, which can be treated as nonresonant isotopes. These isotopes' cross section is generated with infinite dilute background cross section, and they are excluded from the interference treatment. The second category contains the

resonant nuclides, which are included in the interference treatment but with low number densities. These isotopes have hardly any influence on the spectrum of the fuel, but their effective cross section is interfered by the spectrum. Only one point of number density ratio is required for these isotopes for UFG calculation, which is the same order of magnitude as in the fuel. The third category contains the resonant nuclides, which have considerable influence on the spectrum; thus, the interference among these nuclides should be fully addressed. The criterion used to categorize resonant nuclides depends on the actual configuration of the PWR, and the universal criterion should be a compromise between accuracy and efficiency.

In this way, the number of UFG calculation cases are reduced to several thousands. For modern computers, the UFG calculation time of a single fuel pin cell takes less than one second. In a typical PWR configuration, there are only a few types of fuel. To sum up, generating multidimensional RI tables of pseudo isotopes takes a few hours, and it takes less time if the UFG calculation tasks of 1-D heterogeneous cases are parallelized.

To further reduce the calculation time of the interpolation procedure in each resonance self-shielding treatment, a fitting procedure can be used based on the UFG results of the RI tables to obtain the polynomial approximation of Eq. (16), for example,

$$\sigma = A_1T^2 + A_2T + A_3\sigma_b^2 + A_4\sigma_b + A_5\sigma_bT + \sum_i^N (A_{4i+2}D_i^2 + A_{4i+3}D_i + A_{4i+4}D_iT + A_{4i+5}D_i\sigma_b), \tag{17}$$

where N stands for the collection of resonant isotopes, which belong to the third category, and D_i stands for the number density ratio of each resonant nuclide in the third category.

The self-shielded cross section of the pseudo isotope and individual resonant isotope in the mixture can be calculated instantly using the polynomial approximation, and only the coefficients of A are saved in the library for each RI table.

For a typical MOX fuel cell, the relative error of the polynomial approximation is shown in Table III. The results show that most of the errors are under 0.5%, and the polynomial approximation is suitable for modeling the function in Eq. (16). However, it is noted that all the errors are positive, and the accuracy can be further improved. The error of the fitting procedure is mainly caused by the polynomial equation, and the limitations are reflected in the results. Further research on the optimized polynomial equation with better accuracy is ongoing.

IV. NUMERICAL RESULTS

The numerical results of HPRIM coupled with ESSM are shown in this section. To investigate the accuracy of HPRIM, multigroup microscopic effective cross sections are compared with the reference results. Two types of reference results are provided. One type of reference cross section is obtained using a Monte Carlo method in MCNP (Ref. 23). It is a direct approach that includes a rigorous consideration of the resonance interference effect. Another type of reference cross section in pin cell cases is obtained by 1-D UFG slowing-down calculation using the code UFOP. These reference results are consistent with HPRIM because the RI tables of pseudo-resonant isotopes are generated by UFOP. All of the reference cross sections are condensed to the WIMS 69-group structure. The cross sections of groups 22 through 27 are given because all of the resonance isotopes' resolved cross sections are within this range. The multidimensional RI tables of pseudo-resonant isotopes are generated according to the procedure discussed in Sec. III.C.

TABLE III
Relative Error (%) of the Polynomial Approximation for Group Cross Sections

Group ^a	²³⁸ U ^b			²³⁵ U			²³⁹ Pu		
	A	vF	S	A	vF	S	A	vF	S
22	+0.307	+0.238	+0.200	+0.138	+0.112	+0.131	+0.317	+0.221	+0.208
23	+0.453	+0.443	+0.208	+0.163	+0.156	+0.131	+0.422	+0.328	+0.322
24	+0.357	+0.322	+0.259	+0.251	+0.229	+0.131	+0.746	+0.466	+0.210
25	+0.401	+0.396	+0.224	+0.293	+0.281	+0.142	+0.428	+0.411	+0.141
26	+0.155	+0.163	+0.130	+0.374	+0.325	+0.137	+0.489	+0.407	+0.196
27	+0.317	+0.285	+0.148	+0.423	+0.474	+0.140	+0.377	+0.359	+0.142

^aWIMS 69-group structure.

^bA = absorption cross section; vF = fission yield; S = scattering cross section.

IV.A. UO₂ Pin Cell

A typical PWR fuel pin cell is tested. The geometric configuration is shown in Fig. 10, and the material composition is shown in Table IV. The temperature is 300 K.

To show the applicability of HPRIM, several cases are designed by changing the geometric configuration and material composition of the reference pin cell case. The parameters given in Table V are selected as independent variables to generate different cases. The numbers in the right column are the ratios between the parameters of the generated and reference cases in Fig. 10 and Table IV.

Altogether, 28 cases are tested according to Table V. Table VI gives the relative errors of the microscopic cross section for each group and each isotope. The maximum, average, and root-mean-square (RMS) relative errors of all cases are listed in Table VI.

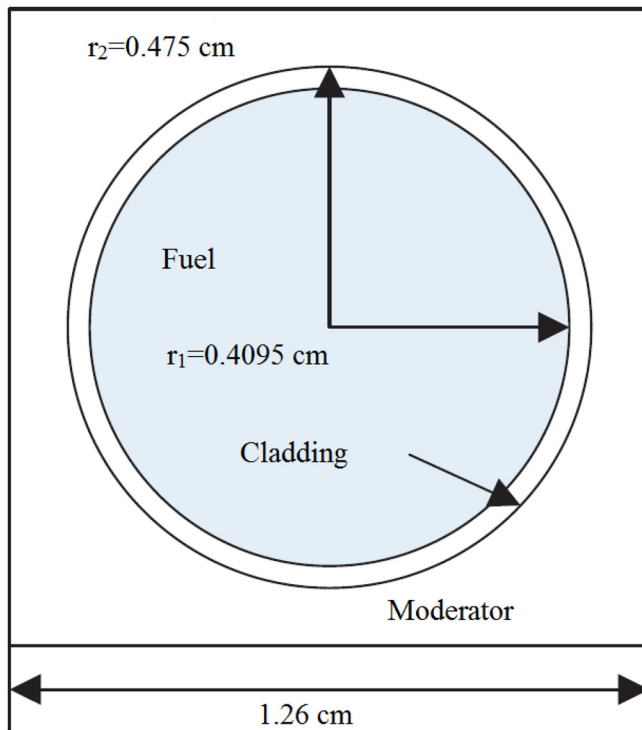


Fig. 10. Configuration of the pin cell problem.

TABLE IV

Material Composition of the Fuel Cell

Material	Atomic Density (10^{24} atoms/cm ³)				
	²³⁸ U	²³⁵ U	¹⁶ O	¹ H	Zr (Natural)
Fuel	0.02194	0.001155	0.04619	—	—
Cladding	—	—	—	—	0.04360
Water	—	—	0.03362	0.06723	—

TABLE V

Ratio of Independent Variables Relative to the Reference Case

Number density of moderator	1, 0.75, 0.5, 0.2, 0.0025
Side length of the cell	1, 1.4, 2, 2.3
Number density of mixture of resonant nuclides	1, 0.5, 0.25, 0.125, 0.0625
Temperature	1, 2, 3, 3.6
Enrichment (linear variation)	1, 2, 3, 4, 5, 6, 7, 8, 9, 10
Enrichment (logarithmic variation)	0.001, 0.01, 0.1, 1, 10, 100

HPRIM is highly consistent with the UFG slowing-down calculation, especially in some extreme cases such as high enrichment. The maximum relative error in each group for each isotope is less than 1.0%, and the RMS relative error is less than 0.2%. HPRIM also shows good accuracy compared to results of MCNP. In some groups, the maximum error of the cross section is about 2%, which indicates that the error is mainly from UFOP. The group structure and collision probability calculation used in UFOP is not good enough for some extreme cases. However, the RMS error is below 1.5%, which indicates that HPRIM exhibits good accuracy in most of the cases. From the aspect of applicability, HPRIM is better than the RIF method because the approximations adopted in the RIF method are avoided or corrected. The errors of the cross sections obtained using the improved subgroup method with RIF correction^{5,6} are also compared with those obtained using HPRIM. In this case, the new subgroup method is improved by a numerical fitting procedure and a scattering model with IR approximation, and the resulting errors in the cross section for the condition of a single resonant isotope are all under 1%. Figure 11 shows the relative errors for the reference case, and Fig. 12 shows the relative errors for a modified case in which in the ²³⁵U enrichment is twice that of the reference case. The solid lines in Figs. 11 and 12 represent the reference microscopic cross sections of ²³⁸U.

Overall, the relative errors of the cross section obtained by the subgroup method with RIF are larger than those of HPRIM. The multiplication factor is also calculated with the resonance cross section obtained by each method. Table VII shows the error in the multiplication factor caused by the calculation of the self-shielded cross section.

The reference results are obtained using the self-shielded cross sections obtained by MCNP. All transport calculations are performed using the MOC solver. It can be seen that the results of HPRIM are very close to those of the UFG slowing-down calculation, and the errors of the subgroup method with RIF correction are larger in both cases.

TABLE VI
Relative Errors of Microscopic Cross Section in All Pin Cell Cases

Group	MCNP as Reference								
	Average			Maximum			RMS		
	U5A ^a	U5vF ^b	U8A ^c	U5A	U5vF	U8A	U5A	U5vF	U8A
22	-0.172%	-0.270%	0.352%	0.493%	0.688%	2.809%	0.235%	0.311%	0.658%
23	-0.086%	0.017%	0.313%	0.576%	0.696%	1.618%	0.233%	0.221%	0.685%
24	-0.175%	-0.220%	1.197%	0.516%	0.533%	2.776%	0.263%	0.309%	1.500%
25	0.251%	0.288%	0.605%	0.669%	0.723%	2.217%	0.358%	0.376%	0.855%
26	0.137%	0.129%	0.024%	0.851%	0.878%	0.788%	0.324%	0.289%	0.241%
27	0.151%	0.128%	0.924%	1.438%	1.821%	4.256%	0.409%	0.479%	1.125%
Group	UFOP as Reference								
	Average			Maximum			RMS		
	U5A	U5vF	U8A	U5A	U5vF	U8A	U5A	U5vF	U8A
22	0.007%	0.006%	0.078%	0.050%	0.051%	0.528%	0.018%	0.016%	0.163%
23	0.017%	0.015%	0.048%	0.345%	0.295%	0.515%	0.063%	0.054%	0.171%
24	0.012%	0.010%	0.093%	0.107%	0.099%	0.411%	0.036%	0.036%	0.165%
25	0.019%	0.015%	0.088%	0.267%	0.258%	0.461%	0.086%	0.083%	0.170%
26	0.013%	0.007%	0.006%	0.268%	0.185%	0.072%	0.086%	0.061%	0.020%
27	-0.006%	-0.022%	0.087%	0.592%	0.775%	0.451%	0.142%	0.181%	0.165%

^aMicroscopic absorption cross section of ²³⁵U.

^b $\bar{\nu}\sigma_f$ of ²³⁵U.

^cMicroscopic absorption cross section of ²³⁸U.

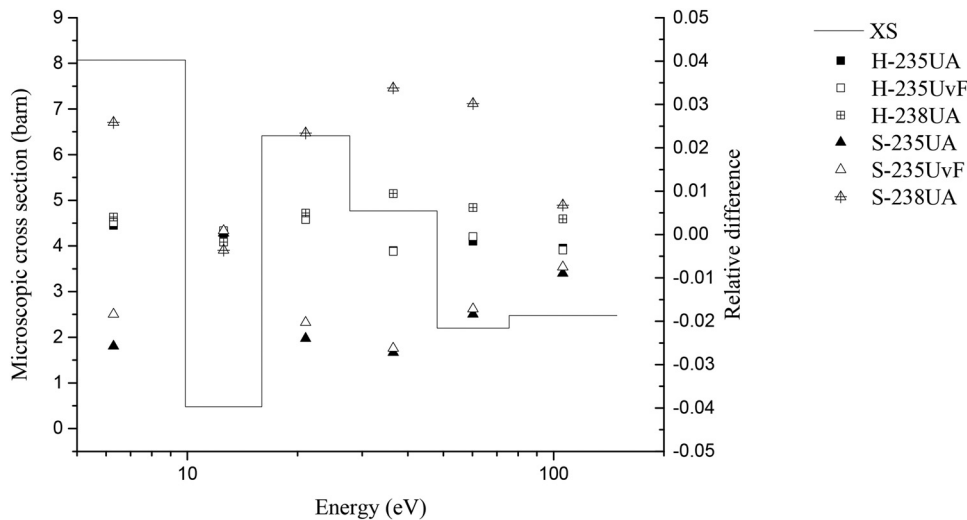


Fig. 11. Relative errors of cross sections obtained by HPRIM coupled with ESSM and subgroup method with RIF correction in low-²³⁵U-enrichment case. H- = HPRIM with ESSM; S- = subgroup with RIF; A = absorption cross section; vF = fission production.

IV.B. MOX Pin Cell

MOX pin cell cases are also tested. Two cases are designed with different plutonium enrichments. The geometric configuration, cladding material, and moderator are

the same as in the previous section, and the fuel composition is shown in Table VIII.

The major resonant absorbers in MOX fuel are ²³⁵U, ²³⁸U, ²³⁹Pu, and ²⁴⁰Pu. The spectrum of the MOX fuel is mainly affected by ²³⁸U, and there is a considerable

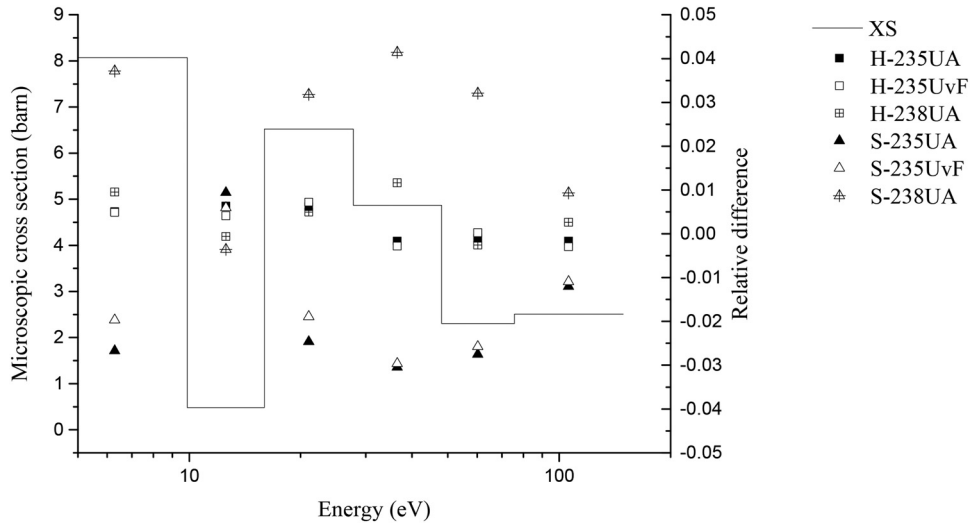


Fig. 12. Relative errors of cross sections obtained by HPRIM coupled with ESSM and subgroup method with RIF correction in high-²³⁵U-enrichment case. H- = HPRIM with ESSM; S- = subgroup with RIF; A = absorption cross section; vF = fission production.

TABLE VII

Comparison of Multiplication Factor Obtained by Different Self-Shielding Methods

Case Description	Multiplication Factor (pcm)		
	UFOP	HPRIM	Subgroup
Low enrichment	-114	-115	-325
High enrichment	-138	-141	-392

TABLE VIII

Material Composition of the MOX Fuel

Nuclide	Atomic Density (10 ²⁴ atoms/cm ³)	
	Low Enrichment of Plutonium	High Enrichment of Plutonium
²³⁵ U	0.001091	0.000917
²³⁸ U	0.020474	0.017197
²³⁸ Pu	0.000046	0.000131
²³⁹ Pu	0.001012	0.002893
²⁴⁰ Pu	0.000482	0.001378
²⁴¹ Pu	0.000175	0.000499
²⁴² Pu	0.000131	0.000375
¹⁶ O	0.046823	0.046777

resonance interference effect among these isotopes. Figures 13 and 14 show the relative errors of the cross sections obtained using HPRIM coupled with ESSM and the subgroup method with RIF correction. The solid lines in Figs. 13 and 14 represent the reference microscopic cross sections of ²³⁸U.

The microscopic absorption cross sections of ²³⁸U, ²³⁹Pu, and ²⁴⁰Pu are examined. For a low-enrichment case, in most energy groups, the errors of the HPRIM treatment are less than 1%, while the errors of the subgroup method with RIF correction are as large as 4%. For a high-enrichment case, the errors of the HPRIM treatment are less than 3%, while the errors of the subgroup method with RIF correction reach 6%. As discussed in Sec. II.B, the error of the RIF method increases with enrichment. The multiplication factor is also compared among different methods. Compared to the reference solution using the self-shielded cross sections obtained from MCNP, the errors in the multiplication factor are around 100 pcm for the UFG slowing-down calculation and HPRIM with ESSM, while those for the subgroup method with RIF are

350 to 470 pcm. It is also observed that the error of the RIF method increases with increasing enrichment.

It is worth noting that all the self-shielding methods in this study are for PWR configurations. In the practical PWR design, the high-enrichment case is rare. The main purpose of including high-enrichment cases in the comparisons in this section and Sec. II.B is to confirm that there are theoretical flaws in RIF theory, and that HPRIM is able to overcome these limitations. The advantages of HPRIM are focused on the MOX cases, which are common in PWR configurations, and the improvements in efficiency are discussed later.

It is also worth noting that in Secs. IV.A and IV.B, it is necessary to demonstrate the accuracy of the subgroup procedure for the condition of a single resonant isotope in order to make a fair comparison.

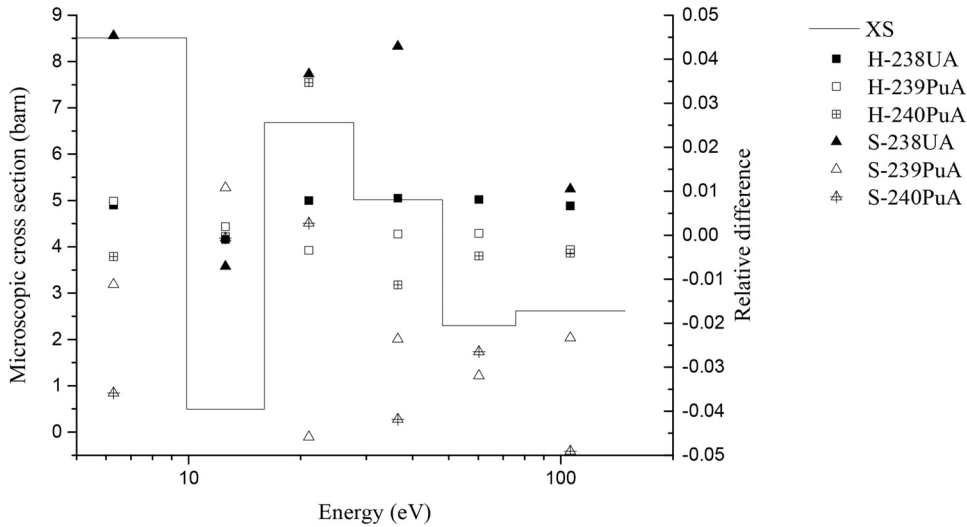


Fig. 13. Relative errors of cross sections obtained by HPRIM coupled with ESSM and subgroup method with RIF correction in low-plutonium-enrichment case. H- = HPRIM with ESSM; S- = subgroup with RIF; A = absorption cross section.

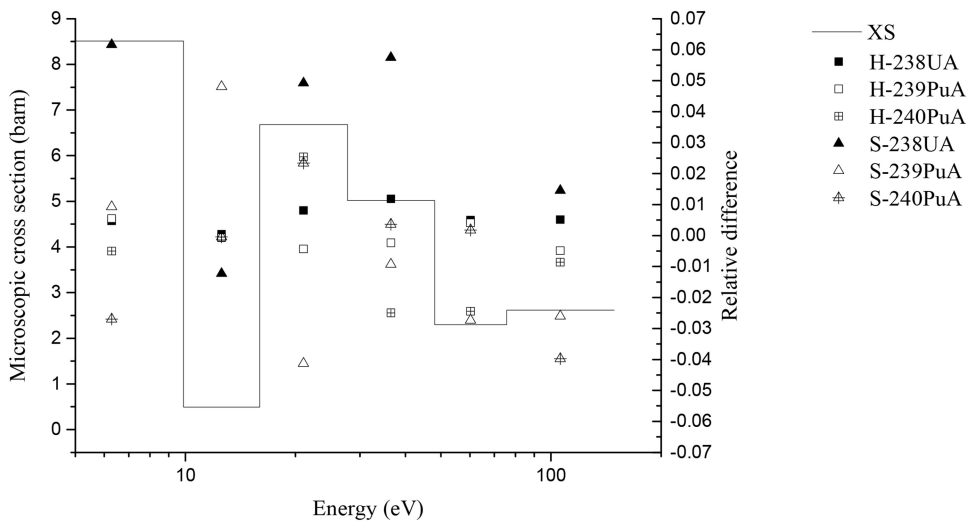


Fig. 14. Relative errors of cross sections obtained by HPRIM coupled with ESSM and subgroup method with RIF correction in high-plutonium-enrichment case. H- = HPRIM with ESSM; S- = subgroup with RIF; A = absorption cross section.

IV.C. Local Heterogeneity

The performance of HPRIM coupled with ESSM is also tested for different local configurations. The four types of geometric configurations are shown in Fig. 15.

The geometric configuration of the fuel pin cell contained in the lattice is the same as in Sec. IV.A. In lattices 1 to 3, the material composition of each fuel pin cell is the same as in the reference pin cell in Sec. IV.A. For lattice 4, there are two types of fuel compositions in the lattice, and two cases are designed. Lattice 4A contains two types of UO₂ fuel. One is the same as the reference pin in

Sec. IV.A, and the other has a reduced enrichment (60% of the enrichment of the reference pin). Lattice 4B contains the UO₂ fuel of the reference case in Sec. IV.A and a low plutonium enrichment MOX fuel in Sec. IV.B. Lattices 1 to 3 show the position-dependent resonance self-shielding effects in a lattice. Lattices 4A and 4B show the interference effects between different fuel pins. Tables IX and X give the relative errors in the microscopic cross sections of individual fuel pins obtained with HPRIM compared to the MCNP results. Table IX shows the errors in the microscopic cross sections of ²³⁵U and ²³⁸U, and Table X shows the errors in the microscopic cross sections

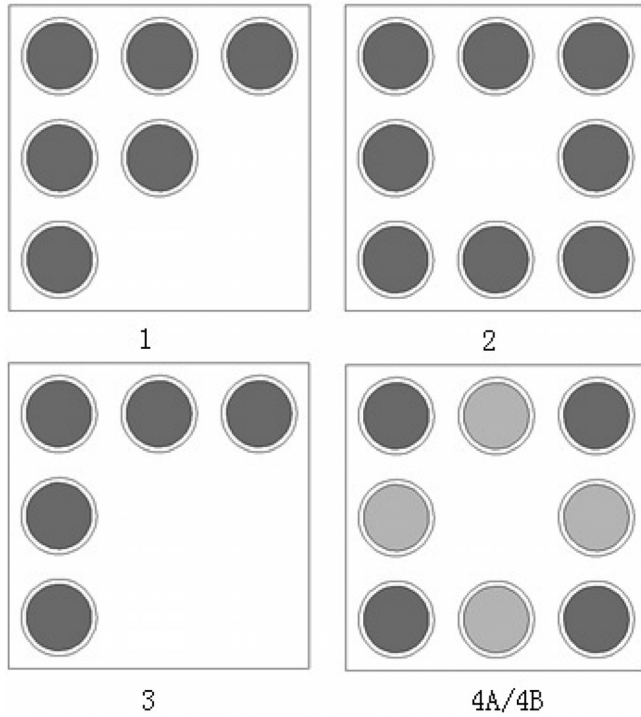


Fig. 15. Configuration of four types of the irregular lattice.

of ²³⁹Pu and ²⁴⁰Pu. The maximum, average, and RMS errors in all the fuel regions of the five lattice configurations are presented.

The RMS errors of the ²³⁸U cross sections are less than 2%, and the RMS errors of the ²³⁹Pu and ²⁴⁰Pu cross sections are less than 5%. The errors in the multiplication factor determined with the computed cross sections are presented for the five lattice configurations in Table XI. The results show that HPRIM captures the local heterogeneity effects with good accuracy, and it can also treat the interference effect among different fuel regions.

IV.D. Efficiency Comparison

As previously discussed, HPRIM treats the entire mixture of resonant nuclides as a pseudo isotope; thus, the self-shielding calculation needs to be done only once, while it is repeatedly performed one by one for all the resonant nuclides in conventional methods. For a large-scale problem, the fixed-source transport calculation to determine the background cross section for each fuel region takes most of the computational effort in the resonance self-shielding treatment. For the UO₂ pin cell case

TABLE IX

Relative Errors of Microscopic Uranium Cross Sections of Individual Fuel Pins of Five Lattice Configurations

Group	Average			Maximum			RMS		
	U5A	U5vF	U8A	U5A	U5vF	U8A	U5A	U5vF	U8A
22	-0.203%	-0.340%	0.013%	0.398%	0.524%	2.997%	0.222%	0.353%	1.208%
23	-0.160%	-0.055%	0.120%	0.503%	0.405%	3.687%	0.226%	0.165%	1.614%
24	-0.267%	-0.309%	1.370%	1.006%	1.098%	2.811%	0.387%	0.422%	1.575%
25	0.190%	0.265%	0.521%	1.160%	1.163%	3.197%	0.384%	0.401%	1.120%
26	0.062%	0.100%	-0.018%	1.578%	1.082%	0.793%	0.664%	0.378%	0.246%
27	0.361%	0.439%	0.565%	1.329%	1.491%	2.574%	0.587%	0.633%	1.225%

TABLE X

Relative Errors of Microscopic Plutonium Cross Sections of Individual Fuel Pins of Five Lattice Configurations

Group	Average			Maximum			RMS		
	P9A ^a	P9vF ^b	P0A ^c	P9A	P9vF	P0A	P9A	P9vF	P0A
22	-1.377%	-1.184%	-1.445%	1.609%	1.466%	1.677%	1.388%	1.200%	1.456%
23	-0.820%	-0.756%	-0.505%	1.044%	0.980%	1.676%	0.839%	0.777%	1.088%
24	-2.943%	-1.525%	-4.259%	3.511%	2.139%	4.612%	2.965%	1.573%	4.292%
25	-2.661%	-2.632%	3.457%	2.913%	2.826%	4.108%	2.668%	2.640%	3.530%
26	-1.138%	-1.084%	-0.046%	1.338%	1.268%	0.058%	1.148%	1.096%	0.047%
27	-1.761%	-1.690%	-0.768%	2.104%	1.993%	0.855%	1.791%	1.716%	0.772%

^aMicroscopic absorption cross section of ²³⁹Pu.

^b $\bar{\nu}\sigma_f$ of ²³⁹Pu.

^cMicroscopic absorption cross section of ²⁴⁰Pu.

TABLE XI

Multiplication Factor Comparison for Heterogeneous Cases

Case	Error in Multiplication Factor (pcm)
1	-83
2	-149
3	-51
4A	76
4B	-17

in Sec. IV.A, Table XII gives the required numbers of fixed-source transport calculations for various combinations of self-shielding methods and interference treatment methods. All the fixed-source transport calculations are performed with the same MOC solver and the same geometric configuration. It shows that HPRIM is the most efficient way to treat the resonance interference effect. The efficiency of HPRIM is more pronounced when a large number of resonant nuclides are involved.

It is also worth discussing the memory usage of HPRIM and the efficiency of RI table preparation. In the preparation of multidimensional RI tables of the pseudo-resonant isotope, a large number of 1-D cylinder cases are calculated by the UFG procedure. Even though the optimized measure in Sec. III.C is taken, the preparation of RI tables for the whole-core-level self-shielding problem can cost several hours of computational time and several gigabytes of memory space. In practice, an independent program that solves the UFG slowing-down equation in parallel is developed to prepare RI tables and transform RI tables to coefficients of the polynomial equation proposed in Eq. (17). For a specific PWR reactor design, the preparation is a one-time job. After the preparation, the self-shielding program can calculate cross sections rapidly using the coefficients of the polynomial equation, which only costs a few megabytes of memory. To further improve the efficiency of the preparation of RI tables and the accuracy of the polynomial equation, the optimized UFG method and improved forms of the polynomial equation are under investigation.

V. CONCLUSION

A detailed analysis of the RIF method in heterogeneous systems is first performed in this paper. The discrepancies in the RIF method are evaluated, and the reasons for the inherent error are discovered. One of these reasons is that the equivalent relationship between homogeneous and heterogeneous cases by background cross section is an assumption that is not suitable for high-enrichment cases. To solve these problems, a new treatment of the resonance interference effect is proposed. The mixture of resonant nuclides is considered as a pseudo-resonant isotope, and the RI of this pseudo-resonant isotope is generated in 1-D heterogeneous cases. The calculation flow of the method and new framework for treating the resonance interference effect are described. The optimized method of generating RI tables for the pseudo isotope is proposed. The advantages of the new method are as follows:

1. high accuracy of resonance interference evaluation due to avoiding the isolated resonant isotope assumption and constant spectrum of the mixture of resonant nuclides
2. strong universality on multigroup resonance self-shielding methods
3. high efficiency over large-scale geometry and mixtures of resonant nuclides that contain large numbers of resonant nuclides.

HPRIM is then coupled with ESSM, and the numerical results show that the new treatment has good accuracy for pin cell cases over a wide range of geometries and compositions. This method can also handle the local heterogeneity effect in the actual lattice physics calculation. The efficiency is superior to other methods. In conclusion, HPRIM is a convenient way to evaluate the resonance interference effect in lattice physics calculation, and it is possible to embed this method into most lattice physics codes to enhance the results of resonance self-shielding.

TABLE XII

Times of Fixed-Source Transport Calculation Performed in Different Methods

Resonance Self-Shielding Methods ^a	RI Iteration Method			Subgroup Method		
	Isotope Iteration	RIF	HPRIM	Isotope Iteration	RIF	HPRIM
Times of fixed-source transport calculation	65	83	30	234	117	39

^aMethods are tested on single pin cell problem. The fuel region contains three resonant isotopes, and the resonance energy group number is 13.

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