M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

The Pseudo-Resonant-Isotope-Model for Predicting the Resonance-Interference Effect in the Self-Shielding Calculation

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Abstract - *The Bondarenko iteration method and the resonance-interference factor have been widely used to predict the resonance-interference effect in the self-shielding calculation. However, these methods not only bring errors into self-shielding results in the specific situation but also cost considerable computational efforts. Pseudo-Resonant-Isotope-Model (PRIM) is proposed to lump the resonances in the resonant mixture to form a pseudo resonant-isotope and generate the resonance integral in the multi-group library. Numerical results show that PRIM is capable of achieving a thorough settlement for the resonance-interference issue with high efficiency by reforming the calculation scheme of conventional self-shielding procedure. It is also a universal technique which can be coupled with many self-shielding methods based on the multi-group structure and it can be easily implemented in the existing or new lattice-physics code. PRIM also has strong potentiality in the large-scale self-shielding tasks such as a direct full-core self-shielding calculation.*

I. INTRODUCTION

The current trend of the reactor-physics calculation is the high-fidelity deterministic calculation on the whole-core level. The resonance self-shielding calculation is a significant part of the lattice-physics calculation and the direct whole-core self-shielding treatment is still one of challenges in high-fidelity deterministic calculation. In the resonance self-shielding calculation of a lattice-physics code, the resonance-interference effect is a long outstanding issue which has been drawing lots of attention and interests from many researchers. The resonance data of each individual resonant isotope is prepared isolatedly in the multi-group library and the detailed resonance-interference information between different isotopes is lost in the multi-group library. In recent decades, the conventional solution toward this issue is the post-treatment on the self-shielded cross sections by direct correction.

In general, there are two types of model to treat the resonance-interference effect. In the early development of lattice-physics codes, such as CASMO-3[1] and DRAGON [2], the Bondarenko iteration[3] was widely used in the self-shielding model based on the equivalence theory. Even though the detail procedures in different codes may vary, the very essence of the model is that only one resonant isotope is considered in the self-shielding procedure while other resonant isotopes are considered as non-resonant at one iteration. The self-shielding procedure goes through each isotope in the mixture and self-shielded cross sections are updated iteratively till convergence. The iteration model is effective in treating the resonance-interference effect in the unresolved energy range, however, non-negligible errors of self-shielded cross sections in the resolved energy range were observed by several researchers [4,5].

In recent researches on the subgroup method[6-8] and Embedded Self-Shielding Method (ESSM)[9,10], the Resonance-Interference-Factor (RIF) method[4] is adopted to obtain better results on the self-shielded cross sections. RIF is the ratio of self-shielded cross sections of a resonant isotope in a homogeneous system between two Ultra-Fine-Group (UFG) calculations: one is that the resonance interference is not considered and the other one is that the resonance-interference effect from other resonant isotopes is explicitly considered while maintaining the same background cross section. RIF is strictly valid in homogenous systems. In practice, the heterogeneous effect is an important issue in the self-shielding calculation of a thermal reactor. However, RIF of the homogeneous geometry has been used intuitively to the heterogeneous geometry without validation. In addition, there are approximations in the RIF calculation and the errors brought by these approximations need to be analyzed as well. Besides the validation of the RIF method, extra computational cost of RIFs is a considerable burden for the self-shielding calculation, especially in large-scale problems with depleted fuel.

The NECP laboratory of Xi'an Jiaotong University (XJTU) have been making efforts to develop resonance calculation methods of high accuracy[11-13]. A Pseudo-Resonant-Isotope-Model (PRIM) based on the Bondarenko iteration and the RIF method has been proposed[5,14], recently.. The model subverts the conventional resonance-interference-treatment procedure by considering the whole resonant mixture as one pseudo resonant-isotope and generating the pseudo Resonance-Integral (RI) table. In other words, the resonance-interference treatment is brought forward before the self-shielding procedure, which makes the resonance-interference treatment an independent task. PRIM is first applied to ESSM to improve accuracy and efficiency[5]. Then PRIM is applied to the subgroup method[14] to enhance the ability of the flexible geometry treatment and capture the sub-ring spatial self-shielding effect.

In this paper, a review of the Bondarenko iteration and the RIF method is made first. Approximations and theoretical flaws of these methods are identified through theoretical derivation and quantitative analysis. . The theories of the PRIM-ESSM and PRIM-subgroup approaches, and the resonance-integral table of the pseudo isotope are described. Numerical results shown that PRIM is a universal technique which can be coupled with many to advance the self-shielding methods calculation and it can be easily implemented in the existing or new lattice-physics codes. PRIM is superior to the Bondarenko iteration and the RIF method from perspectives of accuracy and efficiency. However, PRIM also brings a new challenge in the library preparation for depleted fuel.

II. REVIEW ON CONVENTIONAL METHODS OF TREATING THE RESONANCE-INTERFERENCE EFFECT

1. Bondarenko Iteration

The Bondarenko iteration is proposed based on the Narrow-Resonance (NR) approximation. The spectrum of a resonance mixture can be expressed as:

$$\begin{aligned}\phi_{mix}(E) &= \frac{\lambda\Sigma_{p,mix}+\Sigma_{e,mix}}{\Sigma_{a,mix}(E)+\lambda\Sigma_{s,mix}+\Sigma_{e,mix}} \\ &= \frac{\lambda\Sigma_{p,mix}+\Sigma_{e,mix}}{\Sigma_{a,k}(E)+\sum_{j\neq k}\Sigma_{a,j}+\lambda\Sigma_{s,mix}+\Sigma_{e,mix}}\end{aligned} \tag{1}$$

where the index *mix* stands for the resonant mixture which is a collection of all the resonant isotopes in the mixture, and *k* stands for the target resonant isotope. The information of the macroscopic absorption cross section $\Sigma_{a,mix}$ is not available in the multi-group library, so only one resonant isotope is considered as energy-dependent in the expression. Eq. (1) shows that the background cross section of the target resonant isotope includes absorption cross sections of other resonant isotopes and will be updated during the iteration procedure.

A typical error will be observed in UO_2 fuel composition and it is very common in self-shielding methods using the Bondarenko iteration. For a UO_2 fuel pin-cell case in PWR, relative errors of absorption cross sections of ^{235}U are similar in both the Stamm'ler method[3] and the subgroup method[7] as shown in Figure 1.

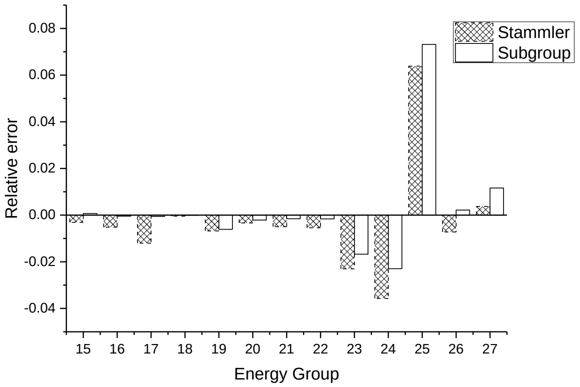


Fig. 1. Comparison of relative errors of absorption cross sections obtained by the Stamm'ler method and the subgroup method

The energy-group structure is the WIMS 69 group[15] and 13 resonance groups （15^{th}~27^{th}）, shown in the appendix, are investigated throughout the paper. Reference results are obtained by the UFG calculation. The largest error occurs at the 25th group and resonances within this group are shown in Figure 2.

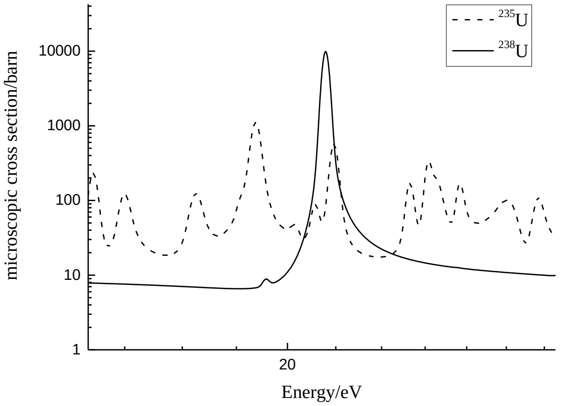


Fig. 2. Resonances overlap within the 25th group

There is a significant overlap of resonances within this group. The mechanism of the error was proved in the early research by a heuristic situation that two resonant isotopes have the same resonance shape[4]. According to Eq. (1), the Bondarenko iteration always have a positive correction on the effective cross section. However, in the heuristic situation, two resonant isotopes having the same resonance shape are equivalent to the situation that one resonant isotope's number density is doubled, which leads to a negative correction on the effective cross section. The contradiction demonstrates that the Bondarenko iteration will lose accuracy when resonances are strongly overlapped. This situation not only happens for ^{235}U in the fresh UO$_2$ fuel but also exists in the depleted fuel when other resonant isotopes are strongly interfered by ^{238}U.

An alternative explanation of the error source of the Bondarenko iteration is that the NR approximation is used in the derivation above. It is well known that the NR approximation is not suitable for wide resonances located in the low energy range of 4 eV -100 eV. When resonances of resonant isotopes are isolated from each other, the model in Eq. (1) is proper while it is not suitable when resonances are interfered by other resonances in the same position.

In summary, the Bondarenko iteration is an effective solution to the resonance interference in unresolved energy range while it is not suitable for resolved resonance interference. The details of resonance interference should be considered in the self-shielding procedure. This requirement is fulfilled by the theory of the RIF method.

2. The RIF method

To consider the detailed information of resonance interferences, RIF is proposed as a correction factor which is defined a ratio of the cross sections between the interfered condition and the i isolated condition. The isolated condition means that the cross section of the target resonant isotope is calculated without considering the interference effect from other isotopes while the interfered condition means that full interference effect is taken into account. Figure 3 shows an example of spectrums in the isolated condition and the interfered condition. Spectrums are obtained in a homogeneous case with and without considering the interference of ^{238}U resonances. The difference between the spectrums shows that the correction of the effective cross sections to account for the interference effect is necessary.

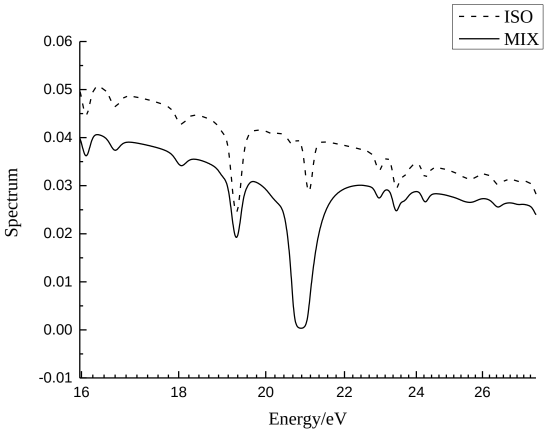


Fig. 3. Comparison of spectrums with and without the interference effect

RIF is defined as

$$f_{x,g}^{k}=\frac{\sigma_{x,g}^{mix,k}}{\sigma_{x,g}^{iso,k}}=\frac{\int\limits_{\Delta E\in g}\sigma_x^k\left(E\right)\varphi^{mix}\left(E\right)\Big/\int\limits_{\Delta E\in g}\varphi^{mix}\left(E\right)}{\int\limits_{\Delta E\in g}\sigma_x^k\left(E\right)\varphi^{iso}\left(E\right)\Big/\int\limits_{\Delta E\in g}\varphi^{iso}\left(E\right)} \quad (2)$$

where the index *mix* and *iso* stand for the interfered condition and the isolated condition respectively. The index *x* stands for the reaction type.

Theoretically, RIF defined above is obtained in the target resonant self-shielding problem, including homogeneous systems and heterogeneous systems. However, it is unpractical to calculate RIF for each problem because it is equivalent to solving the problem directly. To pre-store RIFs or generate RIFs rapidly on-line, in practice, RIF defined by Eq. (2) is usually calculated in homogenous cases. Three important factors affect the value of RIF of the target resonant isotope: temperature, background cross section and concentration ratio of resonant isotopes interfered each other. When RIF is applied to a heterogeneous geometry, temperature and ratio of number densities are known as the input for calculating RIF. However, the background cross section of a heterogeneous region is unknown. An equivalent background cross section to calculate the RIF is inspired by the equivalence theory and it is not only used in the interpolation of RI tables but also used in deciding the correspondent RIF. For subgroup methods without the direct use of the background cross section, the background cross section can be obtained by the inverse-interpolation in the RI table. In summary, the common procedure of the RIF calculation in heterogeneous systems is shown in Figure 4.

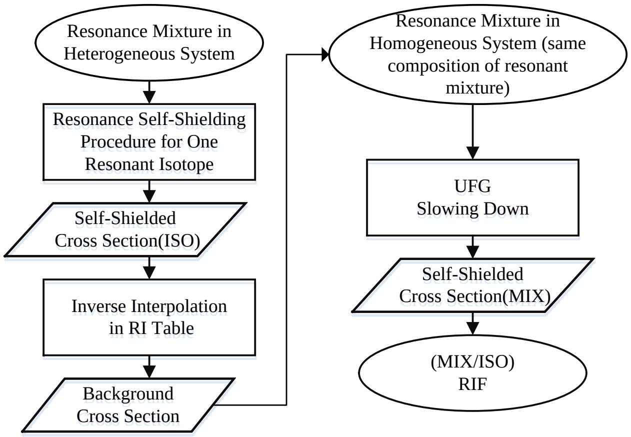


Fig. 4. The common procedure for the RIF calculation

In the beginning of the chart, the two resonance mixtures have the same concentration of resonant isotopes and same background cross section for the target resonant isotope. In other words, the resonance interference in heterogeneous condition is equivalent to the resonance interference effect in homogeneous system as in equivalence theory.

Because the RIF defined in Eq. (2) is rigorously calculated by the UFG method, the RIF correction is time consuming because of large number of UFG calculations for each resonant mixture. Theoretically, the resonant mixture with N types of resonant isotopes need 2×N times of UFG calculations. In researches of the RIF method, two measures are often taken to reduce the computational cost. One is that the spectrum in Eq. (2) is approximated using the analytic form base on the NR approximation[16]. Another one is that RIF is considered between only two resonant isotopes and the secondary effect of interference is neglected, thus RIFs can be pre-tabulated[17].

From theoretical derivation and numerical verification，four possible error sources of RIF have been observed.

Error Source A:

For the RIF method based on the NR approximation, an obvious error source can be located by a comparison between the NR approximation and the UFG calculation.

In author's researches[18,19], the analytic form of the spectrum based on the NR approximation is one of the error sources of the equivalence theory in the resolved energy range. The deviation of the spectrum of the resonant mixture caused by the NR approximation will lead to an error of the RIF calculation, both in homogeneous and heterogeneous systems. A simple test of a homogeneous case with UO_2 is shown in Table I, which gives the relative error of RIF caused by the analytic form of the spectrum based on the NR approximation. The 23rd, 24th, 25th and 27th energy groups (from 4 eV to 75.5 eV) are selected because large resonances are located in these groups. Since Intermediate Resonance (IR) and Wide Resonance (WR) models are also used in the analytic form of the spectrum, relative error of RIFs obtained by IR and WR models are also listed and the reference RIFs are obtained by the UFG calculation. To make the fair comparison, the IR parameter λ for ^{235}U and ^{238}U is both set to 0.2. It is shown that the largest relative error of RIF for ^{238}U obtained by the analytic form of the spectrum based on the NR, IR and WR models is even more than 3% for low energy range.

Table I Relative error of RIFs calculated by IR, WR and NR models

Energy		^{238}U			^{235}U	
group	IR	WR	NR	IR	WR	NR
23	-3.54%	-3.61%	-3.31%	0.35%	0.27%	0.61%
24	-1.49%	-1.56%	-1.26%	-0.24%	-0.44%	0.41%
25	-2.07%	-2.13%	-1.85%	0.43%	0.03%	1.82%
27	-1.56%	-1.66%	-1.20%	-0.22%	-0.83%	1.88%

Error Source B:

For the RIF based on the one-to-one model, the secondary resonance-interference effect is neglected. In a typical LWR fuel pin, ^{238}U has the largest number density and most resonance interferences occur between ^{238}U and other isotopes. Therefore, the one-to-one model is reliable when the resonance interferences from ^{238}U are dominant. However, the mix-to-one model considering all resonance-interference effect should be carried out strictly according to Eq. (2) because the resonance interference is among all resonant isotopes. A simple test can show the differences. A series of homogenous cases with ^{239}Pu, ^{235}U and ^{238}U as resonant isotopes and Hydrogen as the moderator are designed. Background cross section and temperature for ^{239}Pu are kept consistent in each case. RIF for ^{239}Pu is calculated by the one-to-one model and the mix-to-one model respectively. With the one-to-one model, cross sections are corrected with RIF of ^{235}U-^{239}Pu and RIF of ^{238}U-^{239}Pu respectively based on the ". With the mix-to-one model, cross sections are corrected with RIF of mixture-^{239}Pu directly. The comparison is shown in Table II.

Table II Relative difference of RIFs for ^{239}Pu between the one-to-one model and the rigorous mix-to-one model

group	^{238}U:0.02* ^{239}Pu:0.001 ^{235}U:0.001	^{238}U:0.02 ^{239}Pu:0.001 ^{235}U:0.004	^{238}U:0.02 ^{239}Pu:0.001 ^{235}U:0.007	^{238}U:0.02 ^{239}Pu:0.001 ^{235}U:0.01
23	0.132%	0.419%	0.634%	0.809%
24	0.131%	0.356%	0.492%	0.585%
25	0.545%	1.519%	2.134%	2.598%
27	0.282%	0.759%	1.040%	1.252%

*Number density, 10^{24} atom/cm^3.

Relative difference of RIFs for ^{239}Pu in the 25th group is most significant and it increases when the portion of ^{235}U in the mixture increases, which is due to the secondary resonance-interference effect between ^{235}U and ^{238}U. According to the previous investigation, there exist large resonance overlaps in the 25th group. Therefore, the secondary interference is so strong that it cannot be neglected in the calculation of RIF for ^{239}Pu.

Error Source C:

Even though the UFG calculation and the mix-to-one model are both used in the RIF calculation, the accuracy of the RIF still suffers from the error of self-shielded cross section obtained in isolated conditions. Figure 4 indicates that RIF is a function of the background cross section which is a function of the self-shielded absorption cross section obtained in the isolated condition (because the self-shielded cross section at this step will be used in inverse interpolations for background cross sections which are essential on deciding RIFs). For example, for two UO_2 fuel mixtures with different enrichments, RIF for ^{238}U at the 23rd group is shown in Figure 5 as a function of self-shielded cross section obtained in the isolated condition. With the increase of enrichment (with the legend “High” in Figure 5), the trend is more distinct. Error C is caused by the cross-section error predicted by the self-shielding methods in the isolated condition and can be eliminated by improving the accuracy of the multi-group self-shielding methods. This is common in the RIF calculation because in the equivalence theory and the subgroup method, group-wise cross-section prediction errors are common due to different types of approximations involved in these methods.

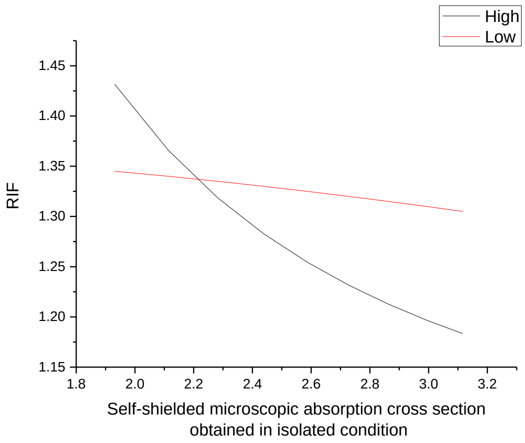


Fig. 5 the relation between RIFs and self-shielded microscopic absorption cross sections in isolated condition

Error Source D:

In the recent trend of the development of self-shielding methods, the UFG method is partially implemented to capture the heterogeneous effect in RI tables[9] or in the self-shielding procedure itself[20]. The ideal situation is that an improved self-shielding model can achieve high accuracy on the cross-section prediction in the isolated condition. It seems that all the error sources mentioned can be eliminated which leads to a complete RIF theory. However, the equivalence relationship between the homogeneous system and the heterogeneous system used in the RIF theory is not validated. Figure 6 shows the differences of spectrums between homogenous cases and heterogeneous cases which are assumed equivalent according to the RIF calculation procedure. “H” and “L” refer to high and low concentration ratio between the target resonant isotops and ^{238}U respectively. The UFG calculation and the mix-to-one model are used and the self-shielded cross section in the isolated condition used for the inverse interpolation is obtained by the UFG calculation to eliminate Error C.

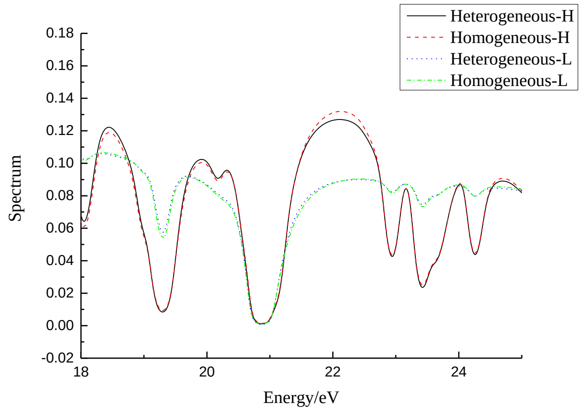


Fig. 6 Comparison of spectrums between equivalent systems

The difference of spectrums between homogenous cases and heterogeneous cases increases with the concentration ratio of ^{235}U in the UO_2 fuel and with the Plutonium concentration in the MOX fuel . Table III and Table IV show the relative difference of RIFs for ^{238}U obtained by spectrums mentioned above in UO_2 and MOX respectively. The 23rd, 24th, 25th and 27th group within 4 eV to 75.5 eV are selected

Table III Relative difference of RIFs for ^{238}U with two calculation procedures for the UO_2 pin cell

group	L[a]	H[b]
23	0.1957%	5.6497%
24	0.5158%	4.1789%
25	0.7294%	5.2368%
27	0.5255%	4.6596%

[a] Low concentration ratio case composed of ^{238}U=0.02, ^{235}U=0.001 (10^{24} atoms/cm^3).

[b] High concentration ratio case composed of ^{238}U=0.02, ^{235}U=0.02 (10^{24} atoms/cm^3).

Table IV Relative difference of RIFs for ^{238}U with two calculation procedures for the MOX pin cell

group	L[a]	H[b]
23	2.4601%	4.5740%
24	1.2360%	1.9208%
25	1.6455%	2.6402%
27	1.7625%	3.0558%

[a] Low concentration ratio case composed of ^{238}U=0.02, ^{235}U=0.001, ^{239}Pu=0.001, ^{240}Pu=0.0005, ^{241}Pu=0.0002, ^{242}Pu=0.0002 (10^{24} atoms/cm^3).
[b] High concentration ratio case composed of ^{238}U=0.017, ^{235}U=0.001, ^{239}Pu=0.003, ^{240}Pu=0.002, ^{241}Pu=0.0005, ^{242}Pu=0.0004 (10^{24} atoms/cm^3).

The results show that the error source D could lead to a 2%~5% relative error of RIFs calculation in high-enrichment cases. The error source is severe because it is an inherent theory flaw in the RIF procedure and cannot be avoided. This type of errors are also observed in sub-ring spatial self-shielding problems[14]. The cross section deviation can reach 20% for ^{238}U. Although in the PWR design, high-enrichment fuel as shown in Table IIIis not common, for MOX fuel and depleted fuel, Error source D is non-negligible for high-fidelity calculation.

All the error sources are reviewed and it is also worth noticing that the RIF method is designed for each target resonant isotope in the resonant mixture, and the RIF correction and the self-shielding procedure will go through all the isotopes. Calculation of RIF y the UFG calculation and the mix-to-one model costs large amount of computational time and memory usage and the self-shielding procedure for each resonant isotope is also a heavy burden for large-scale self-shielding problems with depleted fuel.

From the review of limitations and theoretical flaws of current methods, features of an advanced model to treat the resonance-interference effect are proposed as follows.

(1) The UFG calculation is essential in evaluating the resonance-interference effect on the spectrum of the mixture;

(2) The resonance-interference effect among all the resonant isotopes must be fully addressed;

(3) The assumption of considering only one resonant isotope should be avoided;

(4) The resonance-interference effect should not be confused with the heterogeneous effect and the inherent deviation of the self-shielding procedure.

Thus, a new model of treating the resonance-interference effect is inspired and given in the following parts of the paper.

III. NEW APPROACH FOR TREATING RESOLVED RESONANCE-INTERFERENCE EFFECT

1. Theory

In the Bondarenko iteration derived by Eq. (1), the spectrum can be rewritten as

$$\begin{aligned}\phi_m(E) &= \frac{\lambda\Sigma_p / N_{sum} + \Sigma_{e,mix} / N_{sum}}{\Sigma_a(E)/N_{sum} + \lambda\Sigma_s / N_{sum} + \Sigma_{e,mix}/N_{sum}} \\ &= \frac{\bar{\sigma}_{p,r} + \sigma_0}{\bar{\sigma}_{t,r}(E) + \sigma_0}\end{aligned} \quad (3)$$

$\bar{\sigma}_{p,r}$ and $\bar{\sigma}_{t,r}(E)$ are the average cross sections weighted by the sum of number density of resonant isotopes. From the view point of the continuous cross section within a group, $\bar{\sigma}_{t,r}(E)$ can be taken as the total cross section of a pseudo resonant isotope with new resonance weighted by the number density. For a UO$_2$ fuel, resonances of a pseudo isotope within 4 eV-10 eV are illustrated in Figure 7.

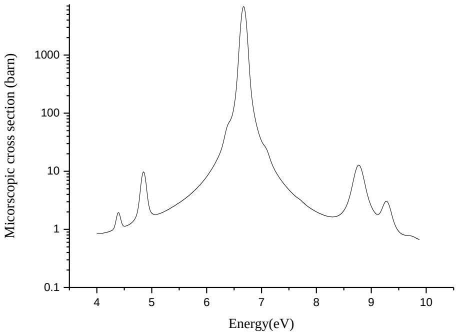


Fig. 7. The illustration of resonances of a pseudo isotope

By constructing a pseudo isotope from a resonant mixture, the resonant mixture which contains the complex resonance-interference effect among resonant isotopes can be equivalent to one pseudo isotope. In this way, during the self-shielding procedure, only one resonant isotope is self-shielded and calculated as a one-time effort without any correction followed.

In practice, pseudo isotope is constructed in multi-group level. The point-wise cross section and scattering kernel of the pseudo isotope are not treated, but RI tables of pseudo isotope are calculated by the UFG calculations on the correspondent resonant mixture. The effective cross section of the pseudo isotope can be defined as

$$\sigma_{x,g}^{pseudo} = \frac{\sum_k N_k \sigma_{x,g}^{mix,k}}{\sum_k N_k} \quad (4)$$

$\sigma_{x,g}^{mix,k}$ is the effective cross section of each resonant isotope directly calculated by the UFG method in homogeneous systems, with the resonance-interference effect considered. The RI tables are prepared by the UFG calculations on different homogeneous systems or heterogeneous systems with different temperatures and background cross sections. In this way, the resonance-interference effect is taken into account and fully addressed in the RI table preparation before the self-shielding procedure so that the downstream self-shielding procedure is independent of interference effect. If PRIM is used in conjunction with the equivalence theory or the subgroup method, the following advantages will be achieved.

(1) Accuracy is improved because the resonance-interference effect is taken into account in the RI table preparation so that many approximations and error sources discussed above are avoided;

(2) High efficiency is achieved due to the simplified procedure. All self-shielding procedures are performed only once because there is only one resonant isotope in the mixture. The efficiency is significantly improved for the large-scale problem with depleted fuel as long as the RI tables of pseudo isotopes are prepared in advance.

2. PRIM-ESSM Approach

Because PRIM is independent of self-shielding methods, the final results of the self-shielding calculation depend on the accuracy of self-shielding methods treating only one resonant isotope. Previous researches have shown that[9,10], the ESSM with 1-D RI tables can achieve high accuracy in the self-shielded cross-section prediction. Therefore, PRIM is first coupled with the ESSM with 1-D RI tables.

The ESSM with 1-D RI tables is based on the one-group fixed-source transport equation:

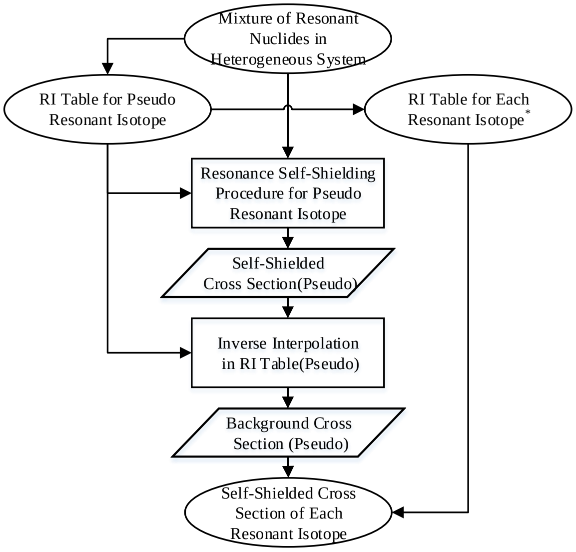
$$\Omega\cdot\nabla\psi_g\left(\vec{r}\right)+\left(\Sigma_{a,g}+\lambda\Sigma_{p,g}\right)\psi_g\left(\vec{r}\right)=\lambda\Sigma_{p,g} \quad (5)$$

and the equivalent background cross section definition:

$$\sigma_{b,g}=\frac{1}{N}\frac{\Sigma_{a,g}\phi_{f,g}}{1-\phi_{f,g}} \quad (6)$$

The initial absorption cross section is used in one-group fixed-source transport calculation and the equivalent background cross section is obtained with the scalar flux calculated. Then 1-D RI tables are interpolated and absorption cross section is updated iteratively till convergence. It is worth noticing that in 1-D RI tables, the RI data is calculated by the UFG method and the background cross section is obtained in the same way as Eq. (5) and Eq. (6). In the ESSM, categorized resonant isotopes or the RIF method is applied for the resonance-interference treatment. However, for PRIM, the whole procedure is very simple: setting up 1-D RI tables for pseudo isotopes constructed in resonant mixture and performing the ESSM for only one pseudo resonant isotope.

At this step, macroscopic cross sections of the resonant mixture can be obtained and used in the transport calculation. However, resonant cross sections of the individual resonant isotope in the mixture is essential in depleted fuel. During the preparation of the RI tables for a pseudo isotope, the RI for each individual resonant isotope can be obtained as the by-product and stored in the library. These data can be taken as the branch RI tables of the pseudo isotope and have the same background cross section defined. These branch RI tables can be used after the equivalent background cross section is obtained by the ESSM. The whole procedure is shown in Figure 8.



*Contain resonance interference effect

Figure 8 Calculation procedure of PRIM.

The PRIM-ESSM approach is very useful for large-scale self-shielding cases with the regular PWR geometry. Self-shielded cross sections of fuel pins can be calculated rapidly if RI tables of the pseudo isotope correspondent to the resonant mixture are generated.

3. PRIM-Subgroup Approach

The PRIM-ESSM approach is able to treat large-scale self-shielding problems with good accuracy and efficiency concurrently. However, a limitation exists in the practical usage. The limitation is that the ESSM itself is not flexible on irregular geometries and sub-ring spatial self-shielding problems. It is well known that the subgroup method is appropriate for flexible geometries. Based on these issues, PRIM is also tested with the subgroup method[14]. The PRIM-subgroup approach focuses on the consistent physical probability table and the subgroup fixed-source equation of the pseudo isotope based on the IR approximation. The effective self-shielded cross sections of the pseudo resonant isotope and the component resonant isotope can be discretized by subgroups as

$$\sigma_{x,k,g}\left(\sigma_b\right)=\frac{\int_{\Delta u_g}\sigma_{x,k}\left(u\right)\frac{\sigma_{\mathrm{b}}}{\sigma_{\mathrm{inter,pseudo}}\left(u\right)+\sigma_{\mathrm{b}}}\mathrm{d}u}{\int_{\Delta u_g}\frac{\sigma_{\mathrm{b}}}{\sigma_{\mathrm{inter,pseudo}}\left(u\right)+\sigma_{\mathrm{b}}}\mathrm{d}u}=\frac{\sum_{i=1}^{I}\frac{\sigma_{x,k,g,i}w_{g,i}\sigma_{\mathrm{b}}}{\sigma_{\mathrm{inter,pseudo},g,i}+\sigma_{\mathrm{b}}}}{\sum_{i=1}^{I}\frac{w_{g,i}\sigma_{\mathrm{b}}}{\sigma_{\mathrm{inter,pseudo},g,i}+\sigma_{\mathrm{b}}}} \tag{7}$$

where the subgroup cross sections and subgroup weights are obtained in a curve-fitting procedure.

The subgroup fixed-source equation of the pseudo resonant isotope can be written as

$$\begin{aligned}&\mathbf{\Omega}\nabla\phi_{g,i}\left(\mathbf{r},\mathbf{\Omega}\right)+\\&\left[N_{\mathrm{pseudo}}\sigma_{\mathrm{t,pseudo},g,i}+\sum_{k\notin\mathbf{R}}N_k\left(\mathbf{r}\right)\sigma_{\mathrm{t},k,g}\right]\phi_{g,i}\left(\mathbf{r},\mathbf{\Omega}\right)\\&=\frac{1}{4\pi}w_{g,i}\left\{\begin{array}{l}N_{\mathrm{pseudo}}\left[\lambda_{\mathrm{pseudo}.g}\sigma_{\mathrm{p,pseudo}}+\left(1-\lambda_{\mathrm{pseudo},g}\right)\sigma_{\mathrm{s,pseudo},g,i}\phi_{g,i}\left(\mathbf{r}\right)\right]+\\\sum_{k\notin\mathbf{R}}N_k\left(\mathbf{r}\right)\left[\lambda_{k,g}\sigma_{\mathrm{p},k}+\left(1-\lambda_{k,g}\right)\sigma_{\mathrm{s},k,g}\phi_{g,i}\left(\mathbf{r}\right)\right]\end{array}\right\}\end{aligned} \tag{8}$$

In the subgroup approach, the Super Homogenization (SPH) correction and the IR approximation are also used to improve the accuracy in self-shielded cross-section calculation in the isolated condition to maintain the accuracy of the subgroup approach for the pseudo isotope. The physical probability table and the subgroup weight are prepared for the pseudo isotope and for all the component resonant isotopes based on the RI tables and the branch RI tables mentioned above. Calculation of the subgroup fixed-source equation is only performed on the pseudo isotope once and weighted flux of the mixture is obtained. Weighted flux is then used to reproduce the self-shielded cross section of each individual isotope.

The PRIM-subgroup approach is very useful in complex geometries and sub-ring spatial self-shielding problems due to the ability of the subgroup method. Since the RI table is calculated in the 0-D condition, the computational cost on the library preparation is less than the PRIM-ESSM approach. However, due to the instability in the generation of the subgroup parameters, accuracy of group-wise subgroup cross section needs to be verified thoroughly on the great variety of pseudo isotopes. On the other hand, a direct subgroup calculation on the large-scale problem costs more computational effort than the ESSM.

4. PRIM RI tables

In both the PRIM-ESSM and PRIM-subgroup approaches, RI tables can always be generated on-line based on the compositions of resonant mixtures. The on-line procedure can be a promising way for future computers. However, for a full-core resonance self-shielding calculation with millions of resonant regions, the practical approach is to pre-generate RI tables for pseudo isotopes.

The multi-dimensional RI table of the pseudo isotope is inspired by the RIF approach. Large amount of tests show that the RI of the pseudo isotope varies monotonically with the number-density ratio of component resonant isotopes. For example, Figure 9 shows the monotonic variation of RI for ^{239}Pu in a resonant mixture of ^{238}U, ^{235}U and ^{239}Pu.

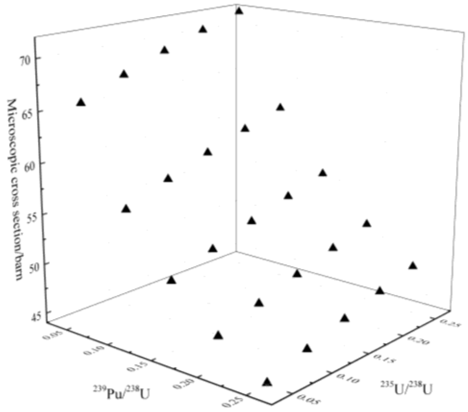


Fig. 9. Monotonic variation of RI for ^{239}Pu with the number-density ratio

The monotonic variation indicates that the cross sections or the RIs of the pseudo isotope and of the component isotope can be a simple function of the number-density ratio between different isotopes. The degree of freedom of the number-density ratio for a resonant mixture with N resonant isotopes is N-1. RI tables can be modeled as,

$$RI=f\left(T,\sigma_b,D_{^{235}U/^{238}U},D_{^{239}Pu/^{238}U},\ldots\right) \tag{9}$$

where

T : Temperature;

σ_b : Background cross section;

D : Number-density ratio vector of each resonant isotope.

With sufficient number of resonant mixture cases, the RI tables can be set up and self-shielded cross sections can be obtained by the interpolation procedure. Furthermore, to reduce the computational efforts and memory usage in the self-shielding procedure, Eq. (9) can be approximated by the polynomial equation,

$$\begin{aligned}\sigma=&A_1T^2+A_2T+A_3\sigma_b{}^2+A_4\sigma_b+A_5\sigma_bT+\\&\sum_i^N\left(A_{4i+2}D_i^2+A_{4i+3}D_i+A_{4i+4}D_iT+A_{4i+5}D_i\sigma_b\right)\end{aligned} \tag{10}$$

Eq. (10) is designed based on the assumption that the dependency between the number-density ratios is neglected. In practice, an independent program is coded to generate RI tables and obtain the coefficients in Eq. (10) by the fitting procedure. In this way, the RI table of a specific pseudo isotope can be generated rapidly and computational cost and memory usage associated with theinterpolation procedure can be avoided. It is worth noticing that Eq. (10) is fitted within a selected range of the number-density ratios. There exist better polynomial equation to cover larger ranges of the number-density ratios.

IV. PRELIMINARY NUMERICAL RESULTS

Numerical results of the self-shielding calculation with the WIMS 69-group structure are shown in this section. A series of PWR MOX pin-cell cases and 3×3 pin-cell cases were tested by the PRIM-ESSM approach. Sub-ring spatial self-shielding problem was tested by the PRIM-subgroup approach. An efficiency test was performed on a full-core self-shielding calculation. Results of self-shielded cross sections are mainly investigated. Results of continuous-energy MCNP[21] calculations are used as reference.

1. MOX pin-cell cases

Two PWR MOX pin-cell cases with different Pu concentrations were tested by the PRIM-ESSM approach and the conventional subgroup approach with the RIF correction. Composition of pin cells are shown in Table V. Group-wise absorption cross section errors are shown in Figure 10 and Figure 11.

The results show that relative errors obtained by PRIM is less than 1% in the low-Pu-concentration case. In the high-Pu-concentration case, relative error in the cross section for ^{240}Pu is about 3% while relative errors for other isotopes are less than 1%. The subgroup method with the RIF correction produces larger relative errors in the self-shielded cross sections: about 5% and 6% for the low- and high-Pu-concentration cases respectively. Errors in the infinite multiplication factor are within 100 pcm for the PRISM-ESSM approach. Errors in the infinite multiplication factor for the subgroup method with RIF reaches are 355 pcm and 478 pcm for the low- and high-Pu-concentration cases respectively. Compared to the RIF method, PRIM is capable of predicting resonance-interference effect with higher accuracy, especially in high-Pu-concentration cases. It is worth noticing that the subgroup data used in this section was carefully tuned so that the error in the self-shielded cross section in the isolated resonant isotope condition is below 1%; and both the UFG calculation and the mix-to-one model were used in the RIF calculation. Thus the error shown in Figure 10 and Figure 11 is mainly caused by the error source D of the RIF method identified in section II.

Table V Material composition of the MOX fuel.

Nuclide	Atomic Density (10^{24} *atom/cm*^{3})	
	Low Pu concentration	High Pu concentration
^{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

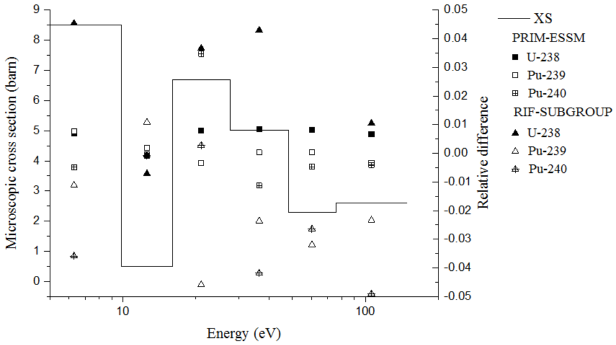


Fig. 10. Comparison of two methods for the low-Pu-concentration case

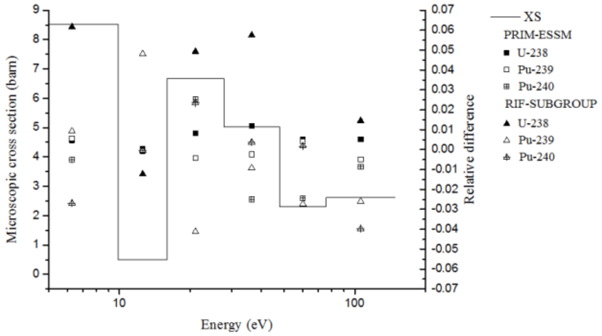


Fig. 11. Comparison of two methods for the high-Pu-concentration case

2. 3×3 pin-cell cases

Local heterogeneous capability of the PRIM-ESSM approach was tested with a few 3×3 pin-cell cases shown in Figure 12.

Case 1 to case 3 is a typical UO_2 fuel with same enrichment. Case 4A consists of two types of UO_2 fuel with different enrichments. Case 4B consist UO_2 and MOX fuels. The moderator in the rest area is water and the boundary condition is all reflective. The temperature in all region is 300K. Table VI gives errors of k_{inf} caused by the resonance self-shielding treatment in the PRIM-ESSM approach.

Table VI errors in K_{inf} caused by the resonance self-shielding treatment in the PRIM-ESSM approach

PWR cases	Error of k_{inf}/pcm
3×3(1)	-83

3×3(2)	-149
3×3(3)	-51
3×3(4A)	76
3×3(4B)	-17

The average, maximum and root-mean-square errors of the absorption cross section of each resonant isotope in each fuel pin for all cases are below 1%. Results show that the PRIM-ESSM approach is valid for heterogeneous problems.

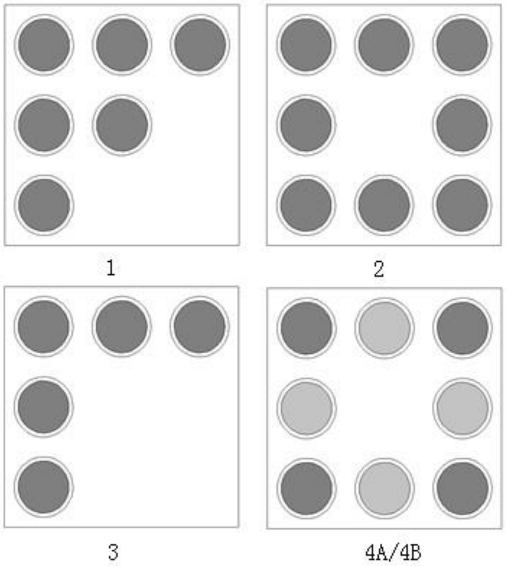
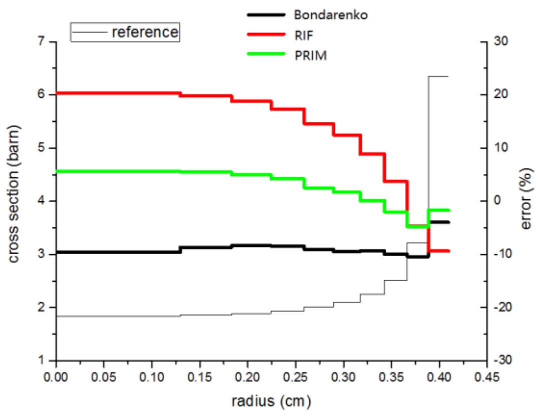


Fig. 12. 3×3 pin-cell layouts

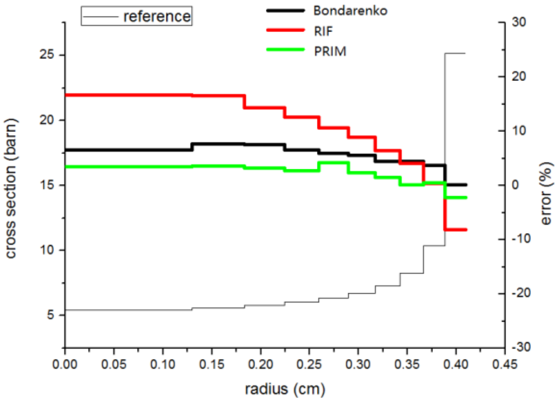
3. Sub-ring spatial self-shielding problem

A typical PWR UO_2 pin cell with the sub-ring geometry was tested by the subgroup approach along with the Bondarenko iteration, RIF and PRIM. Errors for the ^{238}U cross section in the 23rd group and the 27th group along the radial direction of the pin cell are shown in Figure 13.

The comparison shows that PRIM is able to capture the spatially dependent self-shielding effect with good accuracy while errors caused by the Bondarenko iteration and RIF are within 5% to 20%. Errors are larger in the inner rings because the deviation of the spectrum shapes between the inner rings and the homogeneous system is larger. It is noted from Figure 13 that the RIF method is even worse than the Bondarenko iteration, which is due to the error cancelation during the Bondarenko iteration procedure.



(a) 23rd group



(b) 27th group

Fig. 13 Comparison of sub-ring self-shielded cross sections with different methods

4. Efficiency test

A 2-D full-core direct self-shielding calculation was performed to test the efficiency of PRIM. In the self-shielding procedure of large-scale problems, the fixed-source transport calculation is the main computational burden. Efficiency of different methods can be compared by counting the calling times of the fixed-source transport-calculation subroutine. Table VII gives the calling times for the cases of the UO_2 fuel and the MOX fuel.

Table VII Number of calling transport subroutine

	ESSM			Subgroup method(4 subgroups)		
	Bon	RIF	PRIM	Bon	RIF	PRIM
UO_2	65	83	30	312	156	52
MOX	80	249	30	324	468	52

13 resonance groups were calculated and 4 subgroups were used. Results clearly show that PRIM has the fewest

calling times of the transport-calculation subroutine. In the Bondarenko iteration and the RIF method, larger calling times of the transport-calculation subroutine are necessary for each resonant isotope; while in PRIM, only one pseudo isotope is taken into account. PRIM is the most efficient way of treating the resonance-interference effect. Efficiency of PRIM is superior when the number of resonant isotopes is larger, especially for MOX or depleted fuel . It can be concluded that PRIM is specifically designed for large-scale problem with complex resonance interference which are the crucial task in multi-group cross-section preparation for direct full-core calculation. However, this conclusion is based on the fact that the RI tables of all pseudo isotopes are fully prepared and are ready for use. In other word, large amount of computational tasks is brought forward to the multi-group library preparation. PRIM faces the same challenge as the RIF approach when generating large number of tables in advance, especially for the depleted fuel. Better solution towards this issue is under investigation. Fortunately, generating RI tables of pseudo isotopes for a specific core design is a one-time job, that is to say, when RI tables are fully prepared, large amount of computational effort on the whole-core fixed-source transport calculation can be saved with PRIM. The PRIM-ESSM approach is suitable for large-scale problems without considering the sub-ring spatial self-shielding effect while the PRIM-subgroup approach is good the sub-ring spatial self-shielding problem.

V. CONCLUSIONS

A review of the resonance-interference treatment is made in this paper. Based on the error-source analysis, approximations and theoretical limitations are identified for the Bondarenko iteration and the RIF correction. An original technique called PRIM has recently been proposed by the NECP laboratory of Xi'an Jiaotong University (XJTU). PRIM fundamentally changes the original self-shielding framework by lumping resonant isotopes into a pseudo isotope to avoid the possible approximations in the Bondarenko iteration and the RIF correction. PRIM, coupled with ESSM and the subgroup method respectively,was tested with various test cases in this paper. Numerical results show that PRIM is capable of achieving high accuracy with flexible geometrical treatment. Furthermore, PRIM improves the self-shielding efficiency significantly. Features of PRIM is particularly suitable for large-scale problem with complex resonance-interference effect, which is the most crucial issue of the direct full-core resonance self-shielding calculations. Generation of the multi-dimensional library for the depleted fuel is an open problem and the issue is currently under investigation.

APPENDIX: GROUP STRUCTURE OF RESONANT ENERGY GROUPS IN WIMS-69

Energy	Upper boundary/eV
15	9.11800E+03
16	5.53000E+03
17	3.51910E+03
18	2.23945E+03
19	1.42510E+03
20	9.06899E+02
21	3.67263E+02
22	1.48729E+02
23	7.55014E+01
24	4.80520E+01
25	2.77000E+01
26	1.59680E+01
27	9.87700E+00

ACKNOWLEDGMENTS

This work is supported by the National Natural Science Foundation of China Grants No. 11545015 and No.11605128

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