7th International Conference on Modelling and Simulation in Nuclear Science and Engineering (7ICMSNSE)
Ottawa Marriott Hotel, Ottawa, Ontario, Canada, October 18-21, 2015

7ICMSNSE-43

A Fast Resonance Interference Treatment Scheme with Subgroup Method

Liangzhi Cao[a], Qingming He[a], Hongchun Wu[a], Tiejun Zu[a] and Wei Shen[b]
[a] School of Nuclear Science and Technology, Xi'an Jiaotong University, Xi'an, China
[b] Canadian Nuclear Safety Commission, Ottawa, Ontario, Canada
caolz@mail.xjtu.edu.cn, 906459647@qq.com, hongchun@mail.xjtu.edu.cn,
tiejun@mail.xjtu.edu.cn and weishen2010@yahoo.ca

Abstract

A fast Resonance Interference Factor (RIF) scheme is proposed to treat the resonance interference effects between different resonance nuclides. This scheme utilizes the conventional subgroup method to evaluate the self-shielded cross sections of the dominant resonance nuclide in the heterogeneous system and the hyper-fine energy group method to represent the resonance interference effects in a simplified homogeneous model. In this paper, the newly implemented scheme is compared to the background iteration scheme, the Resonance Nuclide Group (RNG) scheme and the conventional RIF scheme. The numerical results show that the errors of the effective self-shielded cross sections are significantly reduced by the fast RIF scheme compared with the background iteration scheme and the RNG scheme. Besides, the fast RIF scheme consumes less computation time than the conventional RIF schemes. The speed-up ratio is ~4.5 for MOX pin cell problems.

Keywords: Resonance Interference Effect, Resonance Interference Factor, Subgroup Method

1. Introduction

Resonance calculation plays an important role in the multi-group approximation based deterministic method. The purpose of the resonance calculation is to obtain the effective self-shielded cross sections for specific problems. Within the resonance energy range, there exist lots of resonance peaks which strongly affect the flux spectrum. Therefore, the scheme of obtaining multi-group cross sections by condensing continuous cross sections with typical flux spectrum is not suitable for the resonance energy range[1]. To treat the self-shielding effects, methods such as equivalence theory[2,3], hyper-fine energy group method[4,5] and subgroup method[6–9] have been developed. The hyper-fine energy group method discretises the energy variable into very fine meshes based on which the neutron slowing down equation is solved. This kind of method treats the energy variable RNGorously and can achieve the same order of accuracy as Monte Carlo method[10]. However, the hyper-fine energy group consumes much computation resources especially for problem of large scale. The equivalence theory typically expands fuel-to-fuel collision probabilities into rational expression in a pin cell model[11]. The equivalence between the pin cell model and a homogeneous model is made based on consistent form of the resonance integral (RI) of the two models. The spatial self-shielding effects are considered through Dancoff correction which takes a blackness assumption of the fuel. The geometrical application of the equivalence theory is limited due to rational approximation. Besides, the accuracy of the method is questionable[12]. The subgroup method discretises a broad energy group into several subgroups according to magnitude of the cross sections. Based on each subgroup, a subgroup fixed source problem (SFSP) is formulated and solved. For the similarity between the SFSP and the multi-group neutron transport equation, mature transport solver such as MOC can be applied. Therefore, the application of the subgroup method is not limited by geometry. This method is widely applied in neutron transport codes such as HELIOS, DeCART and MPACT for its geometrical flexibility and high accuracy.

The procedure of the subgroup method can be divided into two steps. In the first step, the probability tables are generated from the pre-computed RI table; in the second step, the SFSPs are solved to obtain the subgroup flux which is used to obtain the effective self-shielded cross sections. The RI tables are typically obtained by solving neutron slowing down equation of homogeneous system over a range of background cross sections. As the atomic densities of specific problem are unknown, to reduce the disk requirement, the homogeneous system mixes a pseudo background nuclide with only one kind of resonance nuclide rather than multiple resonance nuclides. However, the real problem is not limited to only one resonance nuclide. The resonance peaks of different resonance nuclides will interference with each other which is not considered in the RI table and the subsequent resonance calculation where assumption is made that there is only one resonance nuclide in the system. This discrepancy is the so-called resonance interference effect[13].

The resonance interference effect is conventionally treated by background iteration scheme[14]. In this scheme, resonance nuclides are treated one by one and when the present resonance nuclide is treated, all the others are considered background nuclides which are assumed to be without resonance peaks. Several iterations should be taken to guarantee the convergence of the self-shielded cross sections. There exist two shortcomings in it. Firstly, the iteration procedure is time-consuming especially when there are numerous resonance nuclides. This situation will occur in MOX fuel where six kinds of resonance nuclides exists or in depletion problems. Secondly, the results of iteration can’t converge to the true value[13]. As with the first issue, a Resonance Nuclide Grouping (RNG) scheme was proposed to speed-up the iteration procedure[8,15]. In the RNG scheme, numbers of resonance nuclides are grouped into a small number of categories according to their resonance features. The background iteration is carried out based on the categories rather than each resonance nuclide. Although the calculation efficiency is promoted, it suffers from loss of precision. As with the second issue, the Resonance Interference Factor (RIF) scheme was proposed[13,16–18]. The RIF is the quotient of two sets of self-shielded cross sections, that is, the self-shielded cross sections with a single resonance nuclide without interference and the self-shielded cross sections with the mixture of all nuclides where the resonance interference is fully considered. The RIFs are calculated by continuous energy or hyper-fine energy group method. Then these factors are applied to the self-shielded cross sections without interference obtained by the subgroup method that takes single resonance nuclide assumption. The RIFs can be calculated a priori and tabulated[17], or be generated on-the-fly[19]. However, the scheme to tabulate RIFs a priori increases the storage of nuclear data and the on-the-fly scheme increases the computation time.

In this paper, to overcome the drawbacks of the conventional schemes, a fast RIF scheme is proposed. In this scheme, the dominant resonance nuclide is selected for each resonance group. Then the self-shielded cross sections of the dominant resonance nuclide without resonance interference are calculated by the subgroup method. The heterogeneous system is converted to a homogeneous one by preserving the self-shielded cross section of the dominant resonance nuclide. Finally, the self-shielded cross sections of all the resonance nuclides with resonance interference effect fully considered are obtained by solving the slowing down equation of the homogeneous system in hyper-fine energy group.

The resonance interference treatment schemes as described above have been implemented in SUGAR code[8,9] which employs subgroup method. These four schemes are compared and the results show that the fast RIF is in good agreement with the Monte Carlo method. Besides, the fast RIF scheme shows a promotion in efficiency compared to the conventional RIF scheme.

2. Theory and Model

2.1 Conventional Subgroup Method with the Iteration Scheme

The subgroup method divides a broad energy group into subgroups according to the magnitude of the cross sections. Based on the definition of the subgroup, the subgroup cross sections and the subgroup probabilities are defined as:

$$\sigma_{x,g,i} = \frac{\int_{\Delta E_{g,i}} \sigma_x(E)\phi(E)\mathbf{d}E}{\int_{\Delta E_{g,i}} \phi(E)\mathbf{d}E} \tag{1}$$

$$p_{g,i} = \frac{\Delta E_{g,i}}{\Delta E_g} \tag{2}$$

Based on each subgroup, the Subgroup Fixed Source Problem (SFSP) is formulated:

$$\Omega\nabla\phi_{g,i}(\mathbf{r},\mathbf{\Omega}) + \Sigma_{t,g,i}(\mathbf{r})\phi_{g,i}(\mathbf{r},\mathbf{\Omega}) = Q_{s,g,i}(\mathbf{r},\mathbf{\Omega}) + Q_{f,g,i}(\mathbf{r},\mathbf{\Omega}) \tag{3}$$

Apply Narrow Resonance approximation and ignore the fission source, Eq. (3) can be written as:

$$\Omega\nabla\phi_{g,i}(\mathbf{r},\mathbf{\Omega}) + \Sigma_{t,g,i}(\mathbf{r})\phi_{g,i}(\mathbf{r},\mathbf{\Omega}) = \Sigma_{p,g} \tag{4}$$

Where x is reaction channel; g is broad energy group index; i is subgroup index; $\Sigma_{p,g}$ is potential cross sections. The subgroup cross sections along with the subgroup probabilities are defined as the probability tables. After the probability tables have been obtained, the SFSPs are solved to obtain the subgroup flux which is then used to condense the subgroup cross sections to self-shielded cross sections.

$$\sigma_{x,g}^{\text{eff}}(\mathbf{r}) = \frac{\int_{4\pi}\sum_i \sigma_{x,g,i}(\mathbf{r})\phi_{g,i}(\mathbf{r},\mathbf{\Omega})\mathbf{d\Omega}}{\int_{4\pi}\sum_i \phi_{g,i}(\mathbf{r},\mathbf{\Omega})\mathbf{d\Omega}} \tag{5}$$

The probabilities can be obtained via fitting method or moment method. In this paper, the fitting method is employed which utilizes the RI table to generate the probability tables. For the similarity between the SFSP and the multi-group neutron transport equation, the MOC solver MMOC[20] is used to solve the SFSP.

As the RI tables are obtained based on the assumption that there is only one resonance nuclide in the system, the interference between different resonance nuclides are not considered in the probability tables. Therefore, the assumption is made that there is only one resonance nuclide in the system in Eq. (4) with all the other resonance nuclides considered to be background nuclides. For each resonance nuclide, a SFSP is formulated as:

$$\Omega\nabla\phi_{g,i,k}\left(\mathbf{r},\mathbf{\Omega}\right)+\Sigma_{t,g,i,k}\left(\mathbf{r}\right)\phi_{g,i,k}\left(\mathbf{r},\mathbf{\Omega}\right)=\Sigma_{p,g} \tag{6}$$

Where:

$$\Sigma_{t,g,i,k}=N_k\sigma_{t,g,i,k}+\sum_{k'\neq k}N_k\sigma_{t,g,k} \tag{7}$$

$\sigma_{t,g,i,k}$ is the total subgroup cross section of nuclide *k* of group *g* which is obtained from the pre-generated probability tables; $\sigma_{t,g,k}$ is the total self-shielded cross sections. As the self-shielded cross sections are unknown, an initial guess is used for these cross sections and several steps of iteration are applied to guarantee the convergence of the self-shielded cross sections. At each iteration step, the SFSP is formulated and the subgroup flux are calculated for each resonance nuclide. Then Eq. (5) is applied to update the self-shielded cross sections which are used to obtain the macro total subgroup cross section through Eq. (7). The iteration is terminated when the self-shielded cross sections are converged.

However, there are two shortcomings of this iteration scheme. Firstly, the iteration consumes much computation time to guarantee convergence especially for problems with many resonance nuclides as MOX fuel. Secondly, the converged results are not the true results.

2.2 The RNG Scheme

To cope with the first shortcoming, the RNG scheme was proposed which was adopted by HELIOS[15] and SUGAR[8]. The basic idea is that the numerous resonance nuclides can be grouped into a small number of categories according to the resonance features. To group the resonance nuclides into several categories, all the resonance nuclides are sorted by

$$RS_{k,g}=N_k\mathrm{RI}_{t,k,g}^{\max}/\mathrm{RI}_{t,k,g}^{\min} \tag{8}$$

where $\mathrm{RI}_{t,k,g}^{\max}$ and $\mathrm{RI}_{t,k,g}^{\min}$ are the maximum total RI and minimum total RI of group *g* in the RI table of nuclide *k*, respectively. The quotient of these two values represent the severity of the resonance in the microscopic scale and the $RS_{k,g}$ represents the severity in the macroscopic scale. If the number of categories is *L*, The first $L-1$ resonance nuclides make the first $L-1$ categories and the other make the last category. In the last category, the resonance nuclide with the maximum $RS_{k,g}$ is selected as the typical resonance nuclide. As the values of $RS_{k,g}$ are different for each group, the category of resonance nuclides varies with energy groups.

Within a category of resonance nuclides, the atypical nuclides are considered through the typical resonance nuclide. The subgroup cross section of the whole category is calculated as:

$$\sigma_{l,x,i} = \frac{\sum_{k\in C_l} N_k \sigma_{x,k,i}}{\sum_{k\in C_l} N_k} \approx \frac{\sum_{k\in C_l} N_k \frac{\mathrm{RI}_{k,\infty}}{\mathrm{RI}_{\mathrm{typical},\infty}} \sigma_{x,\mathrm{typical},i}}{\sum_{k\in C_l} N_k} \tag{9}$$

Where l is the category index; C_l is the collection of the nuclide indexes belonging to this category; $\mathrm{RI}_{k,\infty}$ is resonance integral at infinite dilution; N_k is density of nuclide k. Therefore, the whole category of resonance nuclides can be treated as one pseudo resonance nuclide whose subgroup cross sections are calculated by Eq. (9) and subgroup probabilities are inherited from the typical resonance nuclide. The density of the pseudo nuclide is:

$$N_l = \sum_{k\in C_l} N_k \tag{10}$$

After the classification, the background iteration scheme is carried out on the pseudo resonance nuclides. The estimated subgroup flux at the final step of iteration is used to obtain the self-shielded cross sections of the typical resonance nuclide by Eq. (5). The self-shielded cross sections of other resonance nuclides of this category are given by:

$$\sigma_{x,k} = \frac{\mathrm{RI}_{k,\infty}}{\mathrm{RI}_{\mathrm{typical},\infty}} \sigma_{\mathrm{typical},x} \tag{11}$$

In practice, all the resonance nuclides are grouped into two or three categories so that the computation time will be reduced compared to the conventional background iteration scheme. However, as the subgroup flux used to obtain the self-shielded cross sections of the typical resonance nuclide is still based on the iteration, this scheme also suffers from low precision. Besides, as the other nuclides are considered through the typical resonance nuclide, the resonance interference within a category is not considered at all.

2.3 Conventional RIF Scheme

The RIF scheme is promising to address the precision problems of the previous schemes. The basic idea of the RIF scheme is to correct the self-shielded cross section obtained with single resonance nuclide assumption with a quotient of two sets of self-shielded cross sections. The denominator is calculated with single resonance nuclide assumption; the numerator is calculated by fully considering the mixture of the resonance nuclides. The correction equation for the self-shielded cross sections is:

$$\sigma_{x,k,g}^{\mathrm{eff}} = \sigma_{x,k,g} \mathrm{RIF}_{x,k,g} = \sigma_{x,k,g} \frac{\sigma_{x,k,g}^{\mathrm{all}}}{\sigma_{x,k,g}^{\mathrm{single}}} \tag{12}$$

Different from the background iteration scheme, the cross sections of the background nuclides are calculated by:

$$\sigma_{t,g,k} = \sigma_{s,g,k} = \sigma_{p,k} \tag{13}$$

$$\sigma_{a,g,k} = 0 \tag{14}$$

To rigorously obtain the RIFs, continuous energy slowing down calculation is needed. Hyper-fine energy group method or Monte Carlo method is typically used. As the continuous energy calculation is time consuming, much work has been down to improve the efficiency. The first aspect of effort is to calculate the RIFs in an equivalent homogeneous system rather than the heterogeneous system in consideration. Recent work has proven that the homogeneous model can obtain the RIFs at the same level of precision as the heterogeneous model[21]. Although continuous energy calculation of homogeneous system is faster than that of heterogeneous system, it still makes a burden. Based on the first aspect of effort, the second aspect of effort is to tabulate the RIFs a priori against the temperature, dilution cross section and an enrichment-type variable[17]. The tabulation scheme is easily applied to cases where there are only two resonance nuclides, however, it may suffers from huge amount of disk storage for cases with numerous resonance nuclides and is not practical for these cases.

2.4 The Fast RIF Scheme

As the conventional RIF still consumes much computation resources, a fast RIF scheme is proposed. The calculation flow is as follows:

(1) For each broad energy group, the dominant resonance nuclide is chosen according to the magnitude of $RS_{k,g}$ defined in subsection 2.2.

(2) The SFSP is solve for the dominant resonance nuclide with all the other resonance nuclides considered to be background nuclides whose cross sections are calculated by equation (13). Obtain the self-shielded cross sections of the dominant nuclide according to equation (5).

(3) The heterogeneous system is converted to an equivalent homogeneous one. The component of the homogeneous system is all the resonance nuclides in the heterogeneous system and a pseudo background nuclide. The densities of the resonance nuclides are the same with that of the heterogeneous system and the macro dilution cross section is calculated by:

$$\Sigma_{0,g} = \sigma_{0,g} N_{\text{dom}} - \sum_{k' \neq \text{dom}} \sigma_{p,k'} N_{k'} \tag{15}$$

where $\sigma_{0,g}$ is the equivalent dilution cross section obtained by interpolation in the RI tables of the dominant resonance nuclide; N_{dom} is density of the dominant resonance nuclide.

(4) The continuous energy slowing down calculation is performed for the homogeneous system and the effective self-shielded cross sections of all the resonance nuclides are obtained.

In a heterogeneous system, if the number of resonant nuclides is K, the number of spatial mesh with resonance nuclides is M and the number of the resonance groups is G, then the times of SFSP to be solved is G and the times of slowing down calculation is M for the fast RIF scheme. While for the conventional RIF scheme, the times for the above two kinds of calculations are $K \times G$ and $K \times M$, respectively. Therefore, the speedup ratio of the fast RIF scheme against the conventional RIF scheme can be estimated as

$$a = \frac{K \times G \times T_{SFSP} + K \times M \times T_{SDP}}{G \times T_{SFSP} + M \times T_{SDP}} \tag{16}$$

where T_{SFSP} is the time to solve the SFSP and T_{SDP} is the time to solve the slowing down problem.

3. Numerical Results

3.1 Classifying of resonance nuclides

To elucidate the classifying of resonance nuclides in fast RIF and RNG schemes, the values of *RS* defined by Eq.(8) of different nuclides of Mosteller benchmark[22] MOX pin cell problem at Hot Zero Power (HZP) with PuO2 content to be 8% are given in Table 1. As the values of *RS* vary with energy groups, only *RS* for 80th energy group are given. For this group, ^{238}U is selected as the dominant resonance nuclide in the fast RIF scheme as the *RS* is the largest. In the RNG scheme, if the number of categories is three, ^{238}U and ^{239}Pu make the first two categories and ^{240}Pu, ^{241}Pu, ^{235}U, ^{242}Pu make the third group with ^{240}Pu to be the typical nuclide.

Table 1

RS of different resonance nuclides for 80th energy group

Nuclide	Density(atom/b-cm)	*RS*
^{238}U	2.1061e-2	3.9747e-1
^{239}Pu	8.2425e-4	2.1075e-3
^{240}Pu	5.4950e-4	1.3404e-3
^{241}Pu	2.7475e-4	2.8449e-4
^{235}U	1.5275e-4	2.7327e-4
^{242}Pu	1.8317e-4	2.0350e-4

3.2 Comparison of resonance interference treatment schemes

The Mosteller benchmark problems are analysed with different resonance interference schemes. The reference self-shielded cross sections are estimated by OpenMC[23]. To eliminate errors from procedures other than the resonance calculation, the reference k_∞ is calculated using the reference self-shielded cross sections and other cross sections read from the multi-group nuclear library with the transport solver of SUGAR.

The errors of the effective absorption cross sections for MOX pin cell problem at HZP are provided in Figure 1 to Figure 3. The PuO_2 content in the fuel is 8%. It is shown that the errors of the iteration scheme and the RNG scheme are larger than those of the RIF scheme and the fast RIF scheme, especially for ^{240}Pu (Figure 1) and ^{235}U (Figure 2) which are the minor resonant nuclides in the fuel region and are fiercely interfered by the dominant resonant nuclide ^{238}U (Figure 3). The error of the iteration scheme and the RNG scheme is at the same level for the typical resonant nuclides ^{235}U (Figure 2) and ^{238}U (Figure 3). For the atypical ^{240}Pu (Figure 1), the error of these two schemes differentiates from each other largely. The fast RIF scheme and the conventional RIF scheme are in good agreement with the reference.

The time of the resonance calculation, including the time for the SFSP calculation and the slowing down calculation, is compared in Table 2. Compared with the iteration scheme, the RNG scheme groups the six resonant nuclides into three categories and saves half of the time. Compared with the conventional RIF scheme, in the fast RIF scheme, only one resonant nuclide is chosen to perform SFSP calculation and the slowing down calculation are carried out once for all the nuclides rather than for each nuclide. The speed up ratio for the fast RIF scheme given by Eq. (16) is ~4.5. In general, the iteration scheme and the conventional RIF scheme consumes the longest time and the fast RIF scheme consumes the least.

The errors of k_∞ for MOX pin cell problems are compared in Table 3 and results for UO_2 pin cell problems are given in Table 4. For most cases, the RIF and the fast RIF gain higher precision than the iteration scheme. The precision of the RIF and the fast RIF is at the same level. For UO_2 pin cell problems, there are only two resonant nuclides so that there is no atypical resonant nuclide in the RNG scheme. Therefore, the RNG scheme and the iteration scheme are of no difference for UO_2 pin cell problems. For the MOX pin cell problems, the errors of the RNG scheme tend to be cancelled due to overestimation of absorption of ^{238}U and underestimation of absorption of the nuclides of Plutonium.

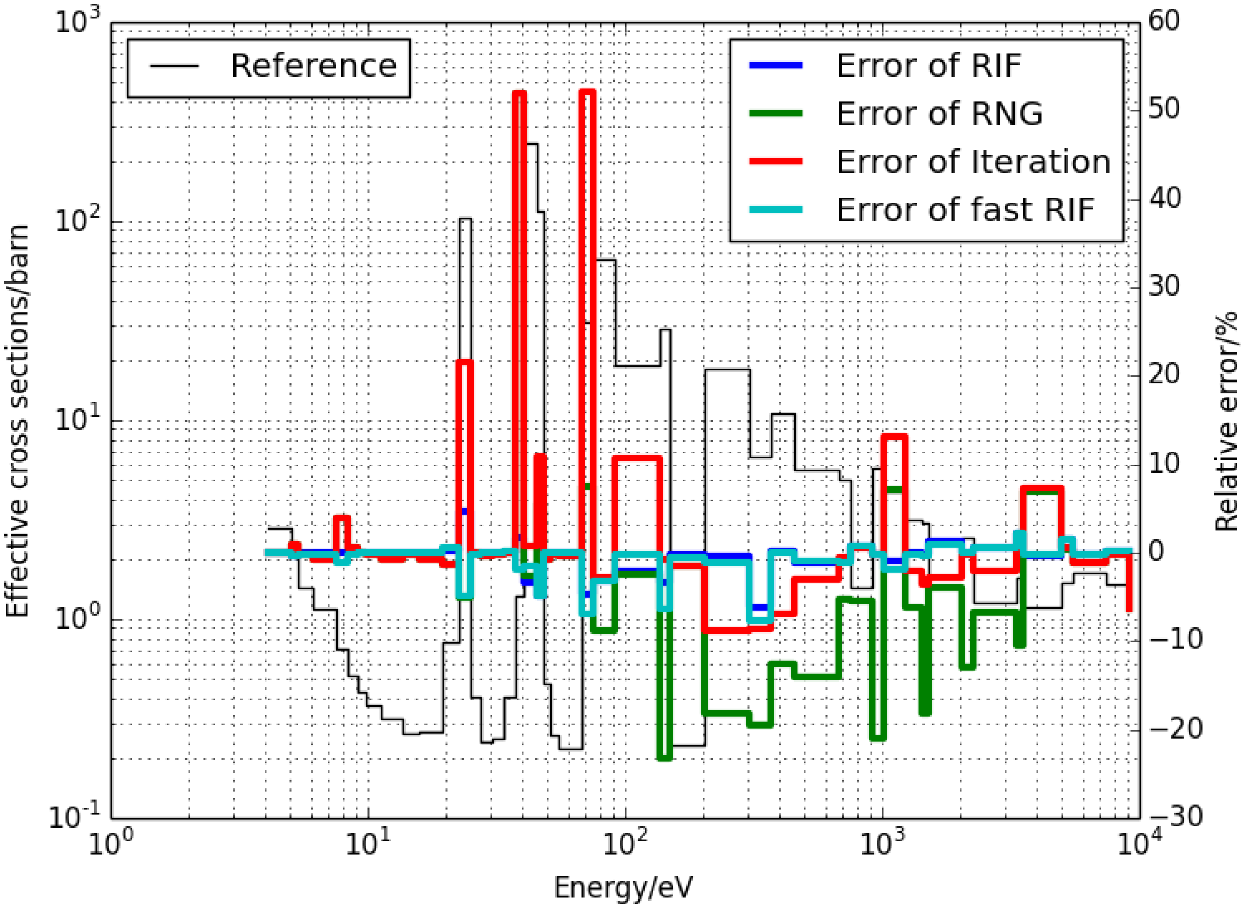

Figure 1 Error of effective absorption self-shielded cross section of different resonance interference schemes for ^{240}Pu

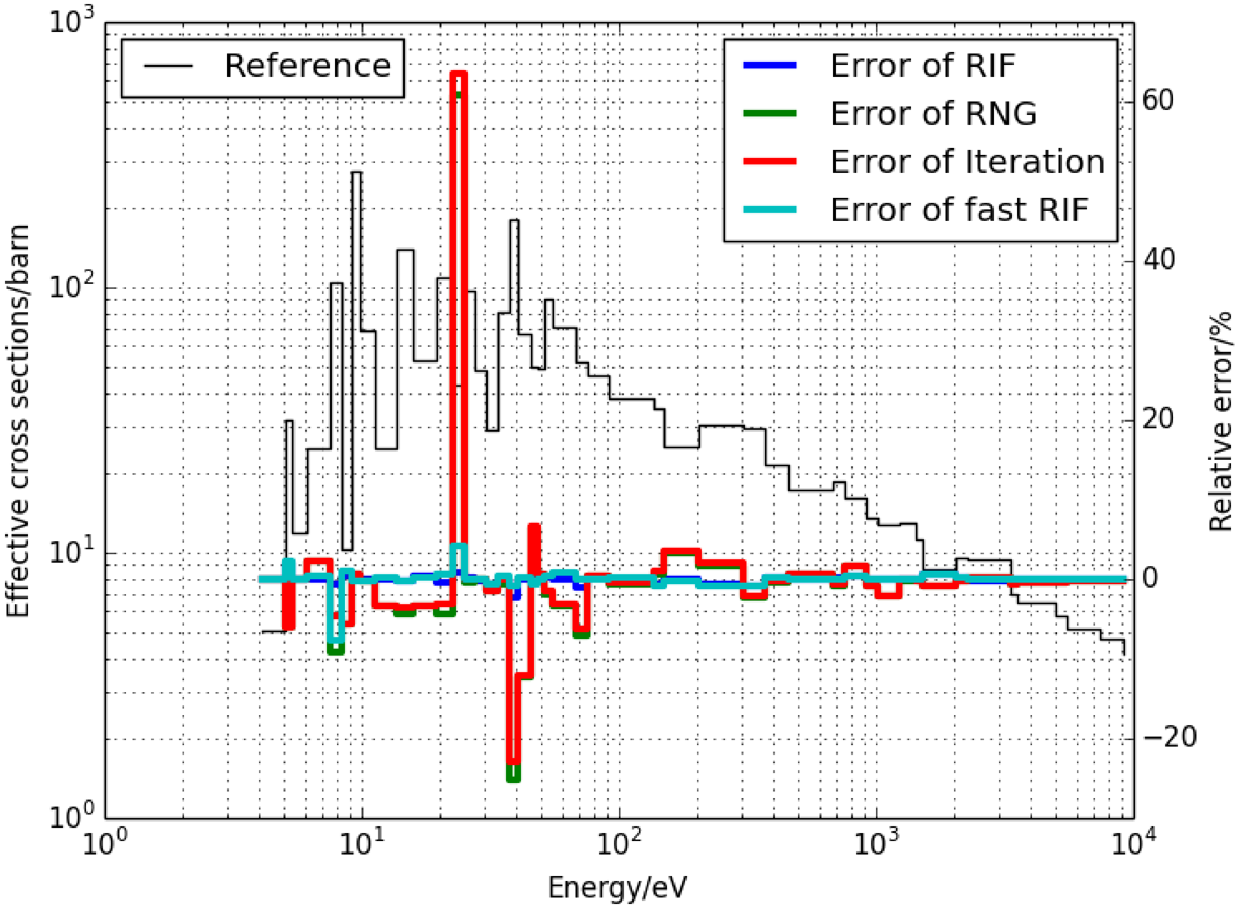

Figure 2 Error of effective absorption self-shielded cross section of different resonance interference schemes for ^{235}U

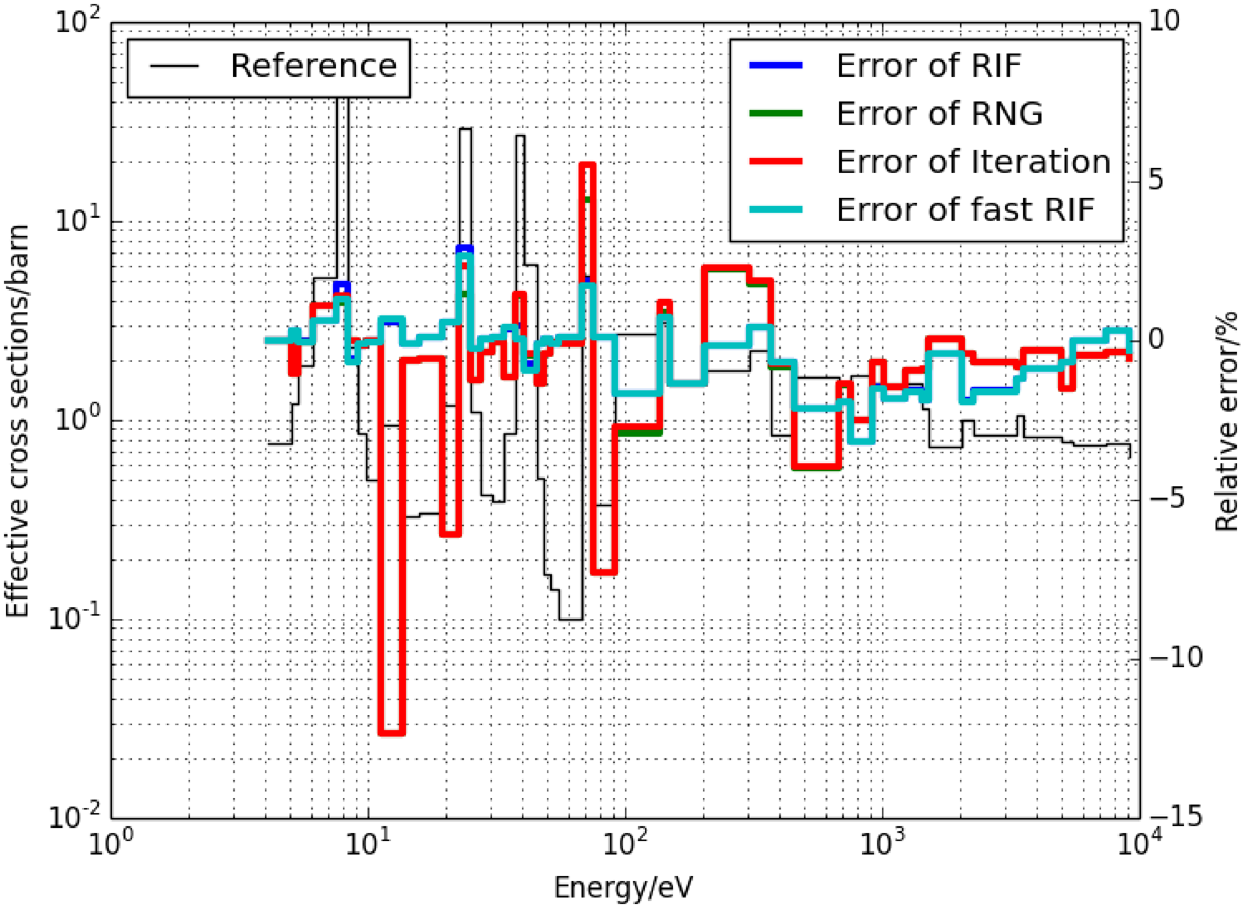

Figure 3 Error of effective absorption self-shielded cross section of different resonance interference schemes for ^{238}U

Table 2

Comparison of time for resonance calculation

Scheme	SFSP/n	SDP/n	Time for resonance calculation/s
Iteration	564	0	108.03
RNG	282	0	55.26
RIF	282	18	106.72
Fast RIF	47	3	23.69

Table 3

Comparison of k_∞ of different resonance interference schemes for MOX pin cell problems

Condition	PuO_2 content (wt.%)	Reference	Error/%			
			Iteration	RNG	RIF	Fast RIF

HFP	1.0	0.93873	-0.14	-0.11	-0.16	-0.12
	2.0	1.01406	-0.17	-0.15	-0.15	-0.13
	4.0	1.06983	-0.21	-0.15	-0.16	-0.13
	6.0	1.09933	-0.24	-0.15	-0.16	-0.14
	8.0	1.12331	-0.27	-0.15	-0.16	-0.15
HZP	1.0	0.94671	-0.14	-0.13	-0.13	-0.10
	2.0	1.02307	-0.16	-0.14	-0.11	-0.09
	4.0	1.07949	-0.20	-0.13	-0.13	-0.11
	6.0	1.10890	-0.21	-0.11	-0.12	-0.11
	8.0	1.13299	-0.25	-0.12	-0.13	-0.13

Table 4

Comparison of k_∞ of different resonance interference schemes for UO_2 pin cell problems

Condition	Enrichment/%	Reference	Error/%			
			Iteration	RNG	RIF	Fast RIF
HFP	0.711	0.66435	-0.11	-0.11	-0.14	-0.10
	1.6	0.95649	-0.13	-0.13	-0.15	-0.14
	2.4	1.09335	-0.14	-0.14	-0.14	-0.11
	3.1	1.17098	-0.16	-0.16	-0.15	-0.13
	3.9	1.23340	-0.17	-0.17	-0.15	-0.13
	4.5	1.26872	-0.18	-0.18	-0.14	-0.12
	5.0	1.29312	-0.19	-0.19	-0.15	-0.13
HZP	0.711	0.66902	-0.12	-0.12	-0.11	-0.09
	1.6	0.96307	-0.14	-0.14	-0.12	-0.12
	2.4	1.10091	-0.15	-0.15	-0.12	-0.10
	3.1	1.17880	-0.16	-0.16	-0.12	-0.10
	3.9	1.24161	-0.18	-0.18	-0.13	-0.11
	4.5	1.27701	-0.18	-0.18	-0.11	-0.10
	5.0	1.30144	-0.19	-0.19	-0.11	-0.10

4. Conclusions

In this paper, the fast RIF scheme is proposed to treat the resonance interference effect and this new scheme is compared with the conventional schemes. The RIF schemes, including the conventional RIF scheme and the fast RIF scheme, estimate effective self-shielded cross sections more accurately. Compared with the iteration scheme, the RNG scheme saves half of the computation time for the MOX pin cell problems. The accuracy of the fast RIF and the conventional RIF scheme is at the same level while the fast RIF scheme consumes much less computation resources. The speed up ratio of the fast RIF scheme is ~4.5 for MOX pin cell problems compared the conventional RIF scheme.

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