

Competitive Resonance Interference Models in Direct Whole Core Transport Code nTRACER

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1. Introduction

nTRACER [1] is a direct whole core calculation code which deals with the local heterogeneity of the core and incorporates the sub-pin level thermal feedback in the single step core calculation at power generating states. It uses its own multi-group (MG) cross section (XS) library that was generated from the ENDF-VII XS data files in a 47 group structure. nTRACER is based on the subgroup method [2] for resonance self-shielding calculations using its own MG library. Recently, the capability of nTRACER was enhanced with WIMS IAEA library [3] using the equivalence theory [4] and Dancoff correction method [5] based on the resonance integral data. The background XSs, for the heterogeneous system, incorporating the shadowing effects, are evaluated by the enhanced neutron current method [5]. The effective XSs are generated using the Resonance Integral (RI) data by interpolating for background XSs and temperatures. The conventional method, which augments the background XS with average absorption XSs of all other resonant isotopes in the mixture, is used for treating the resonance interference in mixed resonant absorbers.

A lot of methods are being developed for the resonance self-shielding in mixed absorbers, but still there exists some inadequacy in the XSs evaluation. The most accurate method is solving the UFG slowing down equation, but at the cost of huge computational burden. On the other hand, the conventional method is the simplest and easy to implement, but it has drawback, that it can't correctly estimate the cross sections in mixed absorbers because it adds the absorption XS. The greater the absorption XS of isotope, the larger will be its contribution on other resonant nuclides in the mixture. This is an iterative procedure to give the converged value for the absorption XSs and hence background XS. So the aim of the present work is to check for the most suitable and effective method in terms of accuracy, execution time and memory usage point of view.

In this paper, the effectiveness of various methods in treating the resonance interference for mixed absorbers is discussed, with the most emphasis on the RIF (Resonance Interference Factors) library method and the microscopic XS table used for RIF generation, the comparison is for these two methods. Both the methods has its pros and cons regarding the efficiency and

accuracy. To see the pros and cons, both the methods are analyzed rigorously. RIF library method will be represented by RIFL while microscopic XS table method will be denoted by XST later in the text.

2. Methodology

2.1 RIF library method

In conventional interference treatment, the effective cross sections are evaluated by taking the background cross section augmented by the average absorption cross section and interpolation of RI data for background cross section. The effective XSs are obtained by the conventional resonance interference treatment as given below [6]:

$$\sigma_x^i = \frac{RI_x^i(\sigma_b^i + \bar{\sigma}_a)}{1 - RI_a^i(\sigma_b^i + \bar{\sigma}_a)/(\sigma_b^i + \bar{\sigma}_a)} \quad (1)$$

where σ_x^i is the effective XS for isotope i , RI_x^i is the resonance integral for reaction x and isotope i , $\sigma_b^i, \bar{\sigma}_a$ are the background XS and average absorption XSs. The average absorption XSs are computed as

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

The conventional interference treatment is not enough to account for the resonance interference because it results in significant errors in the XSs.

In RIF library method, the interference factors are generated for a homogeneous configuration for various background cross sections, energy groups, enrichments and temperatures [6]. With this pre-generated RIF table, the effective XS are determined with no resonance overlap. Then interpolate RIF table for the interference effects of all other isotopes to the target nuclide. The interference from the all other resonant nuclides is added and the perturbations are calculated as given below:

$$\Delta\sigma_{x,g}^r = \sum_{i \in \text{fuel}} [\sigma_{x,g}^r (f_{x,g}^{r \leftarrow i} - 1)] \quad (3)$$

$$\bar{\sigma}_{x,g}^r = \sigma_{x,g}^r + \Delta\sigma_{x,g}^r \quad (4)$$

This method is efficient to estimate the effective cross sections in the mixture with multiple resonant nuclides.

2.2 Microscopic Cross section Table Model

Instead of using the RIF factors table for the number of isotopes, reaction types, enrichments, background cross sections and temperatures with the multi-group library, a method was proposed to use the point wise microscopic XSs for different temperatures and reaction types with the multi group library. To account for the resonance interference, the RIFs are evaluated at the start of each burnup step inside the code for the given composition and the background XS in the homogeneous case. The factors are calculated once per burnup step, so it does not put any extra burden of computations on the code [7]. By definition the resonance interference factors can be written as:

$$f_{RIF}^x = \frac{\sigma_{mix}}{\sigma_{IRW}} \sim \frac{\langle \sigma^x \phi_{mix} \rangle \langle \phi_{IRW} \rangle}{\langle \sigma^x \phi_{IRW} \rangle \langle \phi_{mix} \rangle} \quad (5)$$

where

f_{RIF}^x = RIF for cross sections

σ^x = Mic. Cross sections for reaction x

ϕ_{mix} = Approximate solution corresponding to the mixture dependent flux

ϕ_{IRW} = Approximate solution corresponding to IRW approximation.

$\langle \rangle$ = integration over lethargy

IRW means the ‘‘independent resonance weighting’’ approximation and it states that for each resonant isotope, the multi-group XSs can be evaluated without considering the effect of other resonant isotopes in material on the flux spectrum. In this approximations the resonances are taken as isolated and with no overlap.

The approximate expression can be determined for the mixture dependent and independent resonance approximation fluxes. If all the resonant absorbers are taken to be WR (Wide Resonance) absorbers, then the fluxes can be approximated as given below:

$$\phi_{mix}(u) = \frac{\Sigma_m}{\Sigma_a(u) + \Sigma_m} \quad (6)$$

is the flux for the mixed absorbers, and the IRW flux is given as

$$\phi_{IRW,i}(u) = \frac{\Sigma_m}{\Sigma_{a,i}(u) + \Sigma_m} \quad (7)$$

where

$$\Sigma_{a,i}(u) = N_i \sigma_{a,i}(u) \quad (8)$$

$$\Sigma_a(u) = \sum_{i=1}^{NA} N_i \sigma_{a,i}(u) \quad (9)$$

$$\Sigma_m = \sum_{i=1}^{NM} N_i \sigma_{p,i} + \Sigma_e \quad (10)$$

NA and NM are the number of absorber and moderator isotopes.

Substituting eq. (6) and eq. (7) in eq. (5), it can be obtained:

$$f_{RIF}^x = \frac{\left\langle \frac{\sigma^x}{\Sigma_a(u) + \Sigma_m} \right\rangle \left\langle \frac{1}{\sigma_{a,i}(u) + \sigma_{m,i}} \right\rangle}{\left\langle \frac{\sigma^x}{\sigma_{a,i}(u) + \sigma_{m,i}} \right\rangle \left\langle \frac{1}{\Sigma_a(u) + \Sigma_m} \right\rangle} \quad (11)$$

By using the trapezoidal rule, the integrals in eq. (11) can be evaluated and hence can obtain the RIF factors for the resonance isotopes for a particular reaction.

Microscopic absorption XSs are obtained for uniform lethargy grid for all resonance isotopes at some specific temperature. The number of 20000 grids in the resonance energy range are enough for the resonance interference factors calculations. For uniform lethargy width, the integration is performed within very short time. f_{RIF}^x introduces the resonance overlap for the existence of other resonant nuclides.

3. Verification Results

A homogeneous problem consisting of ^{235}U , ^{238}U , ^{239}Pu , ^{240}Pu and ^1H of the number densities are 2.29918×10^{-4} , 7.34002×10^{-3} , 1.46800×10^{-4} , 1.39460×10^{-5} and 4.46115×10^{-2} #/barn-cm, respectively, is solved to examine the accuracy of the resonance XSs for nTRACER XSs against the MG XS tallied from the corresponding McCARD [8] run. The composition is taken as burned fuel with some concentration of ^{239}Pu and ^{240}Pu . The comparison is made for three methods used in nTRACER with McCARD. Before the XS comparison, the k-eff are first compared for all the three methods as shown in Table I. As noted, the agreement in the k-eff is quite good for the XST and RIFL as compared to conventional. Fig. 1 shows the microscopic absorption XSs for ^{235}U and the relative errors with McCARD results. It is evident from the figure that the most effective method is RIFL which shows quite good agreement with McCARD results. The XST results are also very good as compared to the conventional method but still has large error in lower energy range. Figure 2 shows the microscopic fission XSs for ^{235}U with the relative errors. The figure shows that the errors in the RIFL and XST are quite small as compared to conventional method. Figure 3 shows the microscopic absorption XSs for ^{238}U . The errors in ^{238}U XSs are quite small in this case and the same trend is observed

for the errors. The error for the RIFL are the smallest of all given methods and XST has smaller errors than the conventional method which shows large error. Fig. 4 shows the comparison of the microscopic XSs and %relative errors for ^{239}Pu , which indicate quite good agreement for RIFL which shows minimum error with the reference. XST gives good results than the conventional method but still as large error in some groups. Fig. 5 shows microscopic absorption XSs and relative errors for ^{240}Pu . The figure shows that the XST as well as RIFL both has large errors in some groups while conventional method has very large error. One thing very important is that the accuracy of the RIFL can decrease because in this case the exact RIF are used but XST will behave the same in accuracy. So from these results, it can be deduced that RIFL is very good in accuracy as compared to XST and conventional method while XST is good in accuracy than conventional method but it has some relatively large error in the lower energy group.

Table I: K_{eff} Calculation for homogeneous case

Code	K_{eff}	Reactivity Difference $\Delta\rho$ (pcm)
McCARD	1.31504	-
Conventional	1.30689	-474
RIFL	1.31608	60.1
XST	1.31595	52.6

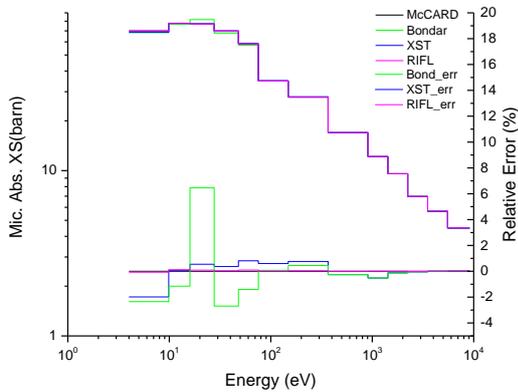


Figure 1: Microscopic Absorption XSs for ^{235}U with Relative Errors

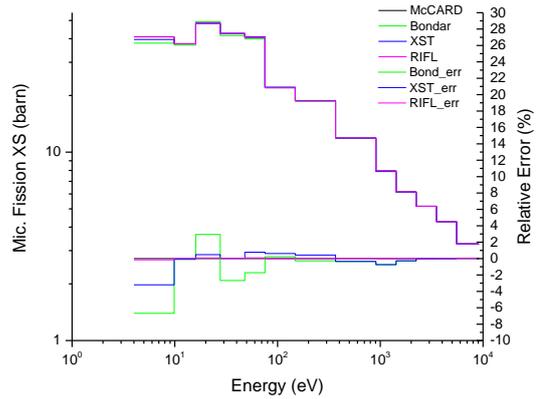


Figure 2: Microscopic Fission XSs for ^{235}U with Relative Errors

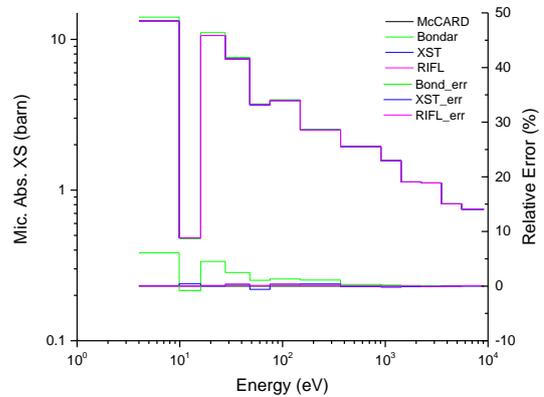


Figure 3: Microscopic Absorption XSs for ^{238}U with Relative Errors

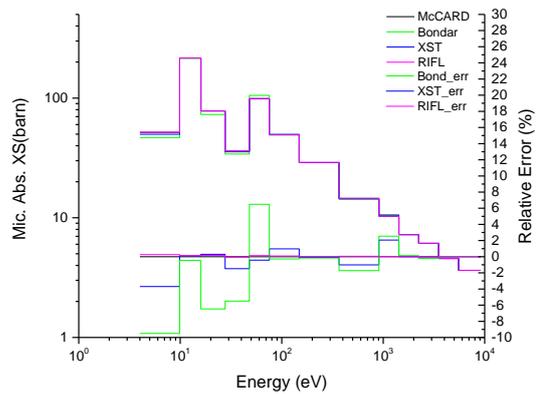


Figure 4: Microscopic Absorption XSs for ^{239}Pu

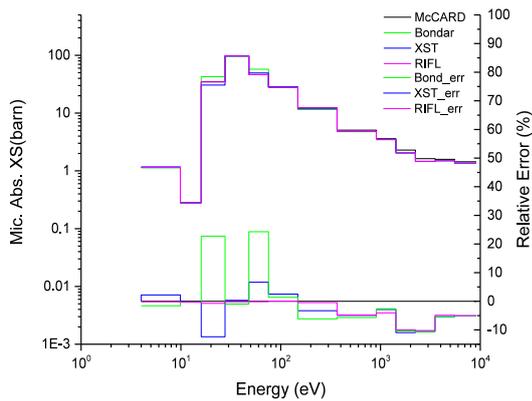


Figure 5: Microscopic Absorption XSs for ^{240}Pu

4. Conclusions

The resonance interference treatment methods are studied and implemented in nTRACER and checked the capacity to improve the overlap effects for multiple resonant isotopes. In XST method, the XSs are improved a lot as compared to conventional method, but still there exists discrepancy in the lower energy range. This method is very fast having no burden during execution. RIFL method is quite good in terms of accuracy and in terms of memory usage, but it increases the computational cost a little which is normally used in table search. In the above analysis exact RIF were used, so the accuracy may decrease by calculating RIF from the contribution of all resonant nuclides on the target nuclide.

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