Generation of Subgroup Weights by Extended Fitting Using Region-wise Resonance Cross Section

Hansol Park, Changhyun Lim and Han Gyu Joo*
Department of Nuclear Engineering, Seoul National University, 1 Gwanak-gu, Seoul, Korea
*Corresponding author: joohan@snu.ac.kr

1. Introduction

The nTRACER [1] direct whole core calculation code being developed at Seoul National University has adopted the subgroup method [2] as a resonance treatment. The subgroup method has been widely used in a commercial light water reactor (LWR) for calculating effective multigroup (MG) cross sections (XS). Among many approaches of the subgroup method, nTRACER adopts the physical probability table approach [3] where heterogeneous effective XSs are pre-calculated over various dilution cases and fitted by the subgroup parameters. For simplicity, only pellet averaged effective XSs are fitted. However, this simplification ignores different behavior of the leakage effect in each subring, and thus, leads to large XS errors in the region-wise sense despite of a small error in the pellet average sense.

In order to resolve this problem, this paper tests two modified fitting schemes: the region-dependent subgroup weights scheme and the extended fitting with region-wise XSs. In the verification section, the comparison of the new methods with the old scheme and the Stoker-Weiss approach [4] in a typical LWR pin-cell problem will be given. The results of the new schemes show great improvement in region-wise XSs. Among the two new methods, this paper suggests the extended fitting method because of its simplicity in the usage phase with the comparable accuracy with the other.

2. Methodology

2.1 Current Limitation of Subgroup Method

The physical probability table approach of the subgroup method fits effective XSs over various dilution cases. In nTRACER, effective XSs are calculated at a typical heterogeneous geometry type of LWR in order to eliminate any bias coming from the difference between homogeneous and heterogeneous geometry. The flux self-shielding expression in the subgroup method resorts to that of the equivalence theory [5] as follow.

$$\phi(u) = \frac{\sigma_b(u)}{\sigma_a^R(u) + \sigma_b(u)}\ , \tag{1}$$

where

$$\sigma_b(u) = \frac{\sum_i \lambda_i \Sigma_{p,i} + \Sigma_e(u)}{N_R}.$$

Please note that, unlike the equivalence theory, the background XS has the lethargy dependency through the escape XS in the subgroup method. And the group condensation is done by the Lebesque integral as follow.

$$\begin{aligned}\int_{u_{g-1}}^{u_g} du\phi(u) &= \int_{u_{g-1}}^{u_g} du \frac{\sigma_b(u)}{\sigma_a^R(u) + \sigma_b(u)} \\ &= \int_{\min_g\{\sigma_a\}}^{\max_g\{\sigma_a\}} d\sigma_a \frac{\sigma_b(\sigma_a)}{\sigma_a^R + \sigma_b(\sigma_a)} \\ &= \sum_{n=1}^{N} \frac{\omega_{a,g,n}\sigma_{b,n}}{\sigma_{a,g,n}^R + \sigma_{b,n}} \\ &= \sum_{n=1}^{N} \omega_{a,g,n}\phi_{g,n}\ ,\end{aligned} \tag{2}$$

where $\sigma_{a,g,n}^R$ is an absorption subgroup level of a resonance isotope, R, in a group g, $\sigma_{b,n}$ is a corresponding subgroup level dependent background XS, $\phi_{g,n}$ is a subgroup flux and $\omega_{a,g,n}$ is a subgroup weight of an absorption subgroup level n.

The flux form of Eq. (1) comes from the conversion of the escape probability to the one term rational form as Eq. (3) in the collision probability transport equation, Eq. (4).

$$P_{esc,f}(u) = \frac{\Sigma_e(u)}{\Sigma_f(u) + \Sigma_e(u)}, \tag{3}$$

$$\phi_f(u) = \frac{Q_f(u)}{\Sigma_f(u)}\left(1 - P_{esc,f}(u)\right) + P_{esc,f}(u), \tag{4}$$

where f denotes a fuel lump in a two-region case and also can represent a sub-region in a multi-region case by assuming the same source driven flux, $Q_j(u)/\Sigma_j(u)$ in all sub-regions inside a fuel. Please note that

Eq. (3) is not described as an approximation, but just a conversion form. This is because the lethargy dependency of a background XS is explicitly considered by solving an explicit transport equation at several subgroup levels. And finally, subgroup based effective XSs are calculated by Eq. (5) over various dilution cases and fitted through subgroup parameters: subgroup levels and weights.

$$\sigma_{eff,x,g} = \sum_{n=1}^{N} \frac{\omega_{x,g,n}\sigma_{x,g,n}\sigma_{b,n}}{\sigma^{R}_{a,g,n}+\sigma_{b,n}} \Bigg/ \sum_{n=1}^{N} \frac{\omega_{a,g,n}\sigma_{b,n}}{\sigma^{R}_{a,g,n}+\sigma_{b,n}}, \quad (5)$$

where x is a reaction type.

Fig. 1 shows the analytic escape probabilities of 15 equi-volumetric sub-rings in a fuel and a fuel lump calculated by using the analytic expression derived in the reference [6]. As shown, such escape probabilities are all different region-by-region so that background XS behaviors in Eq. (3) are all different as an optical length of a fuel lump changes. This means that the relation of effective XS over background XS is different region-to-region. In practice, however, only one relation, i.e. a fuel lump case as the bold black curve in Fig. 1, is used in the fitting process. And in the usage phase, the subgroup parameter set fitted by the fuel lump relation is used in evaluating all region-wise effective XSs.

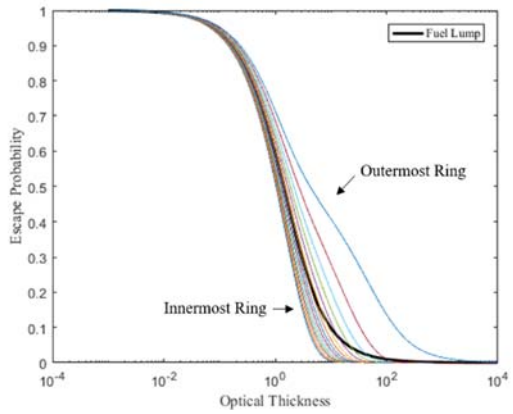

Fig. 1. Analytic escape probabilities of 15 equi-volumetric sub-regions and the total fuel region.

Explaining more physically, the subgroup weight set should be region-dependent in a heterogeneous geometry unlike in a homogeneous one. This is because the subgroup flux, $\phi_{g,n}$, takes part in a different portion in each region and this fact is related to the leakage effect in each region. However, the subgroup weights are generated by taking account of the leakage effect of only a fuel lump. This deficiency of information on region-wise leakage effect over dilutions results in large region-wise effective XS errors, as shown in Fig. 2, in a fuel of a typical LWR pin-cell in resonance groups. 10 dilution cases plus 1 infinite dilution case are used in the fitting [3]. The red bars represent the errors of the pellet averaged XSs and the blue bars are those of the region-wise ones. Apparently, region-wise XS errors are much greater than the pellet averaged XS error which is actually optimized.

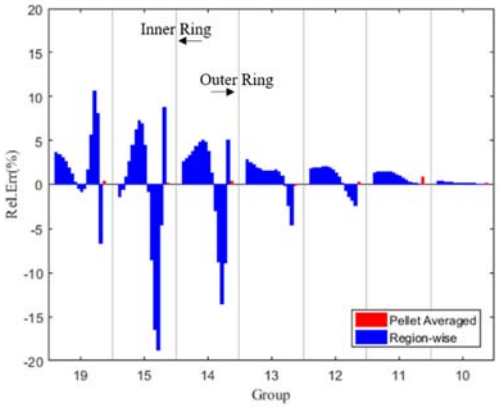

Fig. 2. Region-wise effective XS errors of U238 for the pellet averaged effective XS fitting.

2.2 Extension of Region-wise Effective XS Fitting

Two schemes were tested: the region-dependent subgroup weights scheme and the extended fitting with the use of region-wise XSs. If region-dependent subgroup weights are to be used in order to properly track the physics in play, the original functional to be minimized, Eq. (6) should be changed to Eq. (7).

$$F_g\left(\vec{\sigma}_g,\vec{\omega}_g\right) = \sum_{c=1}^{C}\left(1-\frac{\sigma^{S.G.}_{c,g,F}\left(\vec{\sigma}_g,\vec{\omega}_g\right)}{\sigma^{Ref}_{c,g,F}}\right)^2, \quad (6)$$

$$F_g\left(\vec{\sigma}_g,\left\{f\in F\middle|\vec{\omega}^f_g\right\}\right) = \sum_{f\in F} w^f_g F^f_g\left(\vec{\sigma}_g,\vec{\omega}^f_g\right) = \sum_{f\in F} w^f_g \sum_{c=1}^{C}\left(1-\frac{\sigma^{S.G.}_{c,g,f}\left(\vec{\sigma}_g,\vec{\omega}^f_g\right)}{\sigma^{Ref}_{c,g,f}}\right)^2, \quad (7)$$

where g is a group, c is a dilution case and $\vec{\sigma}_g$ and $\vec{\omega}_g$ are subgroup level and weight sets of Group g, F refers to a fuel lump, f means a subring in a pellet, $\sigma^{S.G.}$ is a reconstructed effective XS by the subgroup method and σ^{Ref} means an effective XS obtained by the ultra-fine group slowing down calculation, respectively. w^f_g is the weight of the target function at each sub-region and the region-wise reaction rate was taken. The optimization was done by utilizing the simulated annealing method [7]. The previous weight

set which reflects only the fuel lump leakage characteristics is now changed to the region-wise subgroup weight sets which consider the leakage effect in its own region.

This approach, however, has complexity of applying a region interpolation of the subgroup weights in the usage phase. In order to detour this difficulty, another fitting scheme, called the extended fitting, was applied as in Eq. (8).

$$F_g\left(\vec{\sigma}_g,\vec{\omega}_g\right)=\sum_{c=1}^{C}\sum_{f\in F}\left(1-\frac{\sigma_{c,g,f}^{S.G.}\left(\vec{\sigma}_g,\vec{\omega}_g\right)}{\sigma_{c,g,f}^{Ref}}\right)^2, \qquad (8)$$

In this scheme, all the region-wise XSs are participated in the one optimization fitting. This unphysical fitting could be possible by taking the most advantage of the non-linear fitting feature with only one set of subgroup parameters per group.

3. Verification

3.1. Problem Description

A normal fresh UO2 pin-cell with the reflective boundary condition was selected. In order to minimize the resonance interference effect, 0.7w/o enrichment was taken. The composition and geometry information is in Table 1. 15 equi-volumetric subrings in a fuel, 32 azimuthal angles in a quadrant, 4 Tabuchi-Yamamoto [8] optimum polar angles in the upper hemisphere and 0.01 ray spacing were used. Inflow P0 transport correction was used and the PSSL method [9] was adopted in order to consider the angle dependency of the resonance MG XSs. As for the resonance interference treatment, the RIFL method [10] was used.

Table 1. Specification of the Pin-cell Problem

	Rad.[a]	Temp.[b]	Nuclide	N.D.[c]
Fuel	0.41	600	U238	2.331867E-2
			U235	1.664843E-4
			O16	4.697031E-2
Gap	0.418	600	He4	2.687140E-5
Clad	0.475	600	Nat. Zr	4.302640E-2
Mod.	1.27 (pitch)	600	H1	4.437307E-2
			O16	2.218653E-2

a) Radius (cm)
b) Temperature (K)
c) Number Density (#/cm-barn)

The new results are compared to the previous subgroup method and also to the S.W. correction. Because this paper examines the intra-pellet region-wise XS accuracy, the lattice effect is considered through the subgroup method and the region-wise effective XSs are adjusted by following.

$$\sigma_{g,f}=\sigma_{g,F}^{S.G.}\frac{\sigma_{g,f}^{S.W.}}{\sigma_{s,F}^{S.W.}}. \qquad (9)$$

3.2. Result and Analysis

Table 2 shows the resulting reactivity errors. In a view of the reactivity prediction, all the methods give allowable results within 100 pcm difference with each other.

Table 2. Pin-cell Reactivity Errors

Code		K-eff	Δρ (pcm)
McCARD		0.88491	±9
nTRACER	S.W.	0.88486	-6
	Old	0.88389	-130
	Ext. Fit.	0.88448	-55
	Reg. Wgt.	0.88401	-115

Before analyzing the reactivity error, the examination on XS error gives meaningful information. Table 3 shows the errors of the U238 pellet averaged XS and Table 4 shows the RMS errors of the U238 region-wise XSs. In the average sense, all methods show small errors less than 1% except the S.W. XS in G19. This is why there's not much reactivity difference each other. However, in the region-wise sense, the S.W. approach and the old one have the inferior intra-pellet region-wise XS accuracy. This poor accuracy is greatly improved by the other two methods. Surprisingly, the accuracy of the extended fitting is as good as the region-dependent subgroup weights scheme despite its unphysical nature of fitting.

Table 3. U238 Pellet Averaged Absorption XS Errors (%) in the Major Resonance Groups

Grp.	S.W.	Old	Ext.Fit.	Reg.Wgt.
10	0.47	0.48	0.46	0.51
11	0.09	0.13	0.04	0.06
12	-0.17	-0.11	-0.30	-0.21
13	-0.31	0.10	-0.31	0.01
14	-0.33	0.73	-0.44	0.58
15	-0.01	0.60	0.12	0.47
19	-2.95	0.46	0.21	0.58

Table 4. RMS Errors* (%) of U238 Region-wise Absorption XSs in the Major Resonance Groups

Grp.	S.W.	Old	Ext.Fit.	Reg.Wgt.
10	1.10	0.48	0.47	0.51
11	3.65	0.32	0.24	0.30
12	4.24	1.48	0.30	0.44
13	4.44	2.44	0.77	0.81
14	4.25	5.86	1.13	0.85
15	5.73	8.11	1.15	0.69
19	6.22	7.47	0.74	0.93

* $\text{RMS Error}=\sqrt{\sum_{f=1}^{N}\left(1-\frac{\sigma_{g,f}^{*}}{\sigma_{g,f}^{Ref}}\right)^2\Big/N}$, N = # of subrings.

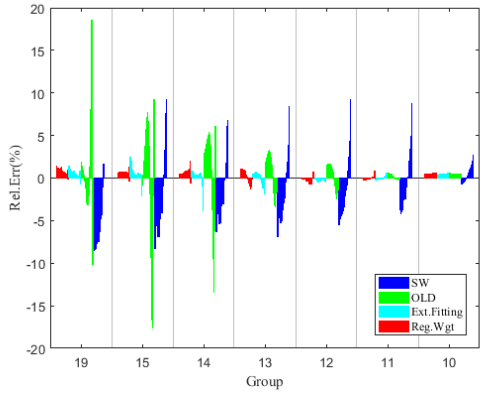

Fig. 3. U238 region-wise absorption XS errors for different approaches in the major resonance groups.

Detailed reactivity error components in a whole pin-cell is given in Table 5. The reactivity errors in Table 5 are calculated by following.

$$Abs. = \left(\Sigma_{a,g,k}\phi_{g,k}^{(n)}V_k\right)^{ref} - \left(\Sigma_{a,g,k}\phi_{g,k}^{(n)}V_k\right)^{'},$$

$$NuF. = \frac{1}{k_{eff}^{ref}} \frac{1}{1 + \frac{1}{\left(\nu\Sigma_{f,g,k}\phi_{g,k}^{(n)}V_k\right)^{'} - \left(\nu\Sigma_{f,g,k}\phi_{g,k}^{(n)}V_k\right)^{ref}}}, \quad (10)$$

where $\phi_{g,k}^{(n)}$ is the normalized flux at Region k of Group g, which gives one total fission source in a given problem.

Table 5. Reactivity Error Components of the Methods

Methods	Thermal	Resonance	Fast
S.W.	-33	26	4
Old	-35	-100	9
Ext. Fit.	-34	-23	6
Reg. Wgt.	-36	-84	8

Considering the XS errors, the good S.W. result is understood as the obvious error cancellation inside a pellet. The 'Old' one is obviously inferior in terms of XS errors which is not predictable due to its randomness. The rest two schemes are comparable with each other and the extended fitting has a small error cancellation from XS errors in Fig. 3 compared to the region-dependent subgroup weights scheme. This is the source of -60 pcm reactivity difference, which is not much meaningful in its quality discussion.

4. Conclusion

The drawback and limitation of the current subgroup method were identified. Due to the different region-wise leakage effects inside a pellet, subgroup weights for the same subgroup level should be different region-wise. However, only one set of subgroup weights considering only a fuel lump leakage effect has been used. Due to this lack of degree of freedom, intra-pellet region-wise XS errors have been large and unpredictable.

The S.W. approach and the two new schemes were tested: the region-dependent subgroup weights scheme and the extended fitting method. The S.W. approach shows very good agreement in its reactivity prediction, which turns out to be from large nice error cancellation. Both the two new schemes show great improvement in the region-wise XS accuracy. However, considering the complexity of the space interpolation of the subgroup weights for the region-dependent subgroup weights scheme, the extended fitting method is thought to be a practical alternative with the similar accuracy.

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