TWO GROUP MICRO-DEPLETION CORRECTION MODEL FOR ALPHA/PHOENIX-P/ANC CODE SYSTEM

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ABSTRACT

A two group micro-depletion method was studied in order to take into account local depletion history, targeting general PWR core design. In this research work, a number density tracking method and a macro cross-section correction method were particulary studied based upon the ALPHA/PHOENIX-P/ANC[1,2] code system currently adopting partially a micro-depletion method, and the validity of these methods was shown from the results of demonstration calculation by the unit assembly calculations.

1. INTRODUCTION

During core design of PWRs, it is very important to take into account local reactivity effects caused by the differences of power history and spectral history at each location in a core. In particular, the importance of considering them has become larger, for various core change in the recent years, such as higher discharge burnup of fuel, longer cycle operation, MOX or recycled uranium fuel application, etc.

In order to take into consideration this local reactivity effect during core calculations, it is necessary to carry out a correction for the macro cross-section of each node according to depletion history during the core calculation. There exist two major approaches for this correction method.

The first method is to determine the correction amount of macro cross-sections for the difference of the history, by the interpolation between macro cross-sections, like CASMO/SIMULATE [3,4] code system. The macro cross-section sets used in the interpolation are generated beforehand with various kinds of histories that can be assumed at local positions in a core.

The other method is a so-called micro-depletion method where the depletion history is expressed by tracking number densities of the major nuclides in a core calculation. In this method, the contribution to the macro cross-section is corrected by using the change of this number density

and the micro cross-section of each nuclide, as partially adopted by ALPHA/PHOENIX-P/ANC code system[1,2].
In order to use the latter method effectively, two requirements should be satisfied, that is, to be able to carry out exactly the number density calculation of each tracked nuclide and to be able to obtain the correct macro cross-section correction based on the number density.
This paper describes the outline of the micro-depletion correction model that is now under development based upon the ALPHA/PHOENIX-P/ANC code system, concerning the latter approach. Simultaneously, it describes a spectral correction model to micro cross-section so as to meet the two requirements mentioned above as well as new depletion technique using 'sub-step' to keep a reasonable depletion step size.

2. MICRO-DEPLETION CORRECTION MODEL

2.1 EXPLICIT TRACKING OF NUMBER DENSITY

In the micro-depletion model discussed here, the nuclides subject to number density tracking are 12 species of actinides shown in Figure 1 and 22 species of fission products shown in Figure 2. On the selection of the nuclides, those that have large contribution to the reactivity were finally selected, as the result of an investigation of importance of each nuclide to fuel reactivity. PHOENIX-P, a 2-D transport calculation code, and a 70-group cross-section library that is based upon ENDF/B-VI were used in this investigation.
As shown in Figure 1, the actinide depletion chain consists of two independent chains. One chain starts from U234 and reaches U236, and the other starts from U238 and reaches Am243. Both of chains are forward chains that change in the direction from parent to daughter, and the feedback from daughter to ancestor does not occur. Accordingly, the number density of each actinide nuclide can be determined by solving simple matrix equations for each chain.
As for fission products, the isotopes of Pm, Sm, Eu and Gd can be treated as one chain, and the other nuclides including Xe can be also as another chain. Both of the chains can be treated as forward chains similar to that of actinides, as shown in Figure 2. However, as it is required to consider the fission yield, a proper transformation of the matrix is necessary to solve the matrix equations. Furthermore, as for the Gadolinia fuel, it was distinguished from the Gd nuclide as the fission product and was treated as the different chain, because it is required to consider spatial shielding effect appropriately.
As for the depletion of each nuclide, the number density was calculated by using two-group flux, two-group micro cross-section, decay constant and fission yield in the nodal calculation and further using reasonable depletion step size by predictor-corrector method. However, in the case of Gadolinia fuel, where the micro absorption cross-section changes largely against the burnup due to spatial shielding effect, this method may not be sufficient. Thus, a special depletion method was adopted for Gadolinia fuel. This is described in Section 4.
In any case, the key points for accurate number density calculation are whether the two-group micro cross-section used in the calculation is adequate or not, and, whether adequate depletion step size is adopted for each depletion step or not. As for the micro cross-section for calculating number density is described in Section 3.

2.2 CORRECTION TO MACROSCOPIC CROSS-SECTION

In this micro depletion model, it is assumed that the macro cross-section sets depending on burnup are used for the core calculation code of ANC. These macro cross-section sets are obtained by the unit assembly calculation that assumes typical condition so as to represent the core, such as nominal power and typical boron concentrations, using a multi-group 2-D transport calculation code like PHOENIX-P. In other words, the contribution of each nuclide in the assumed typical condition is included in the macro cross-sections.
Now, if an actual number density for nuclide *i*, $N_{i,actual}$, reflecting the depletion history at each node in a core is obtained by the above-mentioned number density tracking, here can be written the difference of the contribution to the macro absorption cross-section of the nuclide *i* at the interested node, that is, the correction amount, as follows:

$$\sigma_{ag,i}^{eff}\left(N_{i,actual} - N_{i,ref}\right) \quad , \quad (g=1,2)$$

When the correction is carried out for all the tracked nuclides, the macro absorption cross-section of the concerned node taking into consideration the actual history, Σ_{ag}^{actual}, can be determined as follows:

$$\Sigma_{ag}^{actual} = \Sigma_{ag}^{ref} + \sum_{i} \sigma_{ag,i}^{eff}\left(N_{i,actual} - N_{i,ref}\right) \quad , \quad (g=1,2)$$

Where Σ_{ag}^{ref} is the macro absorption cross-section assuming the typical condition, $N_{i,ref}$ is the number density of nuclide *i* in this condition, and $\sigma_{ag,i}^{eff}$ is the effective micro cross-section obtained by the correction as follows:

$$\sigma_{ag,i}^{eff} = \sigma_{ag,i}^{ref} \times f\left(SI\right) \quad , \quad SI = \phi_1 / \phi_2$$

The factor, *f=f(SI)*, is a correction factor to take into account the difference between the spectrums in the typical condition and in the actual condition, and becomes important especially for the thermal group. This is described in Section 3.
Furthermore, here the absorption cross-section was taken as an example, and, it is actually specified that, as for the actinides, the correction is carried out both for the absorption cross-section and for the fission cross-section, and as for the fission products it is done only for the absorption cross-section.

3. SPECTRAL CORRECTION FOR MICROSCOPIC CROSS-SECTION

It was previously mentioned that the micro cross-section plays an important role in both part of the number density calculation and the macro cross-section correction of each nuclide.

In this section here is described the study to obtain a suitable micro cross-section in each part.

3.1 MICRO CROSS-SECTION FOR NUMBER DENSITY CALCULATION

It is needless to mention again that the micro cross-section consistent with the actual neutron spectrum should be used, in the case the number density is tracked for each nuclide. Currently, the micro cross-section is given as the burnup dependent table in ANC code, similar to the macro cross-section. Since this micro cross-section is obtained assuming the typical core condition, this needs to be corrected corresponding to actual spectrum.

In this research work, it was aimed at to obtain approximately the micro cross-sections, σ_{ag}^{actual} and σ_{fg}^{actual} (g=1, 2), which are near to the actual conditions, from σ_{ag}^{ref} and σ_{fg}^{ref} (g=1,2), the micro cross-sections of each nuclide in the above-mentioned typical condition. Concretely, defining ϕ_1 / ϕ_2, the ratio of the fast neutron flux to the thermal one as spectral index (hereafter called SI), it was investigated whether the ratio of each micro cross-section SGR (=$\sigma_{ag}^{actual} / \sigma_{ag}^{ref}$ or $\sigma_{fg}^{actual} / \sigma_{fg}^{ref}$), can be correlated with the spectral index ratio SIR (=SI_{actual} / SI_{ref}), or not. In this investigation, in order to cover core conditions in a range as wide as possible, 11 kinds of conditions as shown in Table I were handled, and the micro cross-section and the spectral index of each condition were determined from the unit assembly calculation by PHOENIX-P code.

Figure 3 and Figure 4 show the results of investigation for the micro absorption cross-section (thermal group) of U235 and thermal fission cross-section of Pu239, respectively. From these figures, it is understood that a good correlation with SIR has been obtained for the micro cross-section ratio. The fitting curve in the figures is a quadratic one determined by the least square fitting of all plotted points. When the SGR determined from this fitting curve is compared with each plotted point, the difference between them is within approximately 2 % even at the maximum. On the contrary, when this correction is not applied, an error of approximately 5 % can be observed for largely different spectrum from nominal condition.

As a result of the similar investigation also for other nuclides that are objective of number density tracking, it was confirmed that a good correlation with SIR can be obtained for the thermal group micro cross-section ratio, similar to U235. In other words, the thermal group micro absorption cross-section and fission cross-section to be used for the number density tracking regarding nuclide i can be approximately determined using the correction factor SGR utilizing the spectral index, as follows:

$$\sigma_{a2,i}^{actual} = \sigma_{a2,i}^{ref} \times SGR_{a2,i}(SIR)$$
$$\sigma_{f2,i}^{actual} = \sigma_{f2,i}^{ref} \times SGR_{f2,i}(SIR)$$

On the other hand, the similar study was also conducted for the micro cross-section of the fast group. It can be essentially considered that the fast group micro cross-section depends on the neutron spectrum and the fuel effective temperature. However, a good correlation could not be obtained for SI or SIR, even if only the spectrum was changed by changing the boron concentration and by fixing the fuel temperature. Since the contribution in fast group is smaller than that in thermal group in particular for PWR, in this study, it has been assumed that SGR

does not depend on SIR, but is equal to 1.0 for the fast group micro cross-section. Of course, for better accuracy, more detailed study for fast group is required, also including the correlation with the fuel effective temperature.

3.2 MICRO CROSS-SECTION FOR MACRO CROSS-SECTION CORRECTION

As mentioned in Section 2.2, when the following equation is used in macro cross-section correction:

$$\sum_{ag}^{actual} = \sum_{ag}^{ref} + \sum_{i} \sigma_{ag,i}^{eff} (N_{i,actual} - N_{i,ref}), (g=1,2)$$

The micro cross-section, σ_{ag}^{eff}, is intuitively in the middle between σ_{ag}^{ref} and σ_{ag}^{actual} that was determined in Section 3.1. However, essentially, correction may not be only for the changed portion of the number density, but the concept to correct all of contributions of each nuclide is more suitable, like the following:

$$\sum_{ag}^{actual} = \sum_{ag}^{ref} + \sum_{i} (\sigma_{ag,i}^{actual} N_{i,actual} - \sigma_{ag,i}^{ref} N_{i,ref}), (g=1,2)$$

We obtained already the micro cross-section in the actual condition in Section 3.1. Therefore, if only the number density can be exactly obtained, the correct macro cross-section can be approximately reproduced in the actual condition using this correction equation for the remainder.

3.3 VALIDATION

The above-mentioned spectral correction model was incorporated into a core calculation code, ANC, for the testing purpose, and it was confirmed that this spectral correction model is appropriate by running several test cases.
PWR unit assembly geometry (Westinghouse type, standard 17 x 17) was used for all cases. The macro cross-sections and the micro cross-sections were passed to ANC via ALPHA/PHOENIX-P code, assuming the nominal power condition and the constant condition of boron concentration of 500 ppm. Taking this as the base condition, each test case by changing the boron concentration or the power condition was analyzed with / without the spectral correction model added to micro-depletion model. And the number density of each tracked nuclide as well as the fuel reactivity was compared with the reference analysis results by PHOENIX-P for the same conditions. The list of the tested cases is shown in Table II.
Figure 5 shows the changes of the number densities of major actinides due to depletion for Case A0. This is the nominal case where the unit assembly was calculated in the completely same condition as that of the macro cross-section generation. Thus, the number densities obtained with this model are close to them with reference calculation in this figure. Figure 6 shows the comparison of the errors of each number density at 20 GWd/t for the same case. We can see less than 2% error even for higher isotopes in this figure. From these figures, it is clarified that the change of the number density due to depletion can be correctly tracked by the adoption of the

micro-depletion method for the case where the depletion histories are completely the same. Figure 7 and Figure 8 show the comparison of the errors of each number density at 20 GWd/t from the results of the number density tracking in Case A1 and Case A2. Case A1 is the case assumed to be different spectrum condition by changing boron concentration to 1000ppm and Case A2 is the case of different depletion power level. From these figures, it is also clarified that the change of the number density due to depletion can be correctly tracked by the adoption of the micro-depletion method and the spectral correction model even for the case where the depletion histories are different.
Figures 9 to 11 show the comparison of the errors of the infinite multiplication factor, k-inf, due to depletion for Cases A0 to A2. From these figures, it is clarified that the reactivity calculation is accurately carried out for the fuels with various depletion histories, by the application of the micro-depletion method with the spectral correction model.

4. ACCURATE NUMBER DENSITY TRACKING WITH SUB-STEP TECHNIQUE

4.1 SUB-STEP DEPLETION TECHNIQUE

For majority of nuclides, the number density calculation with high accuracy is possible by using the θ-weighting method or the predictor-corrector method, as the neutron flux and the micro cross-section do not largely vary within the depletion step. The neutron flux and the micro cross-section before and after each depletion step are used in this calculation with the depletion step size of approximately 2 GWd/t. However, in the special case such as that of Gadolinia fuel, effective micro absorption cross-section of Gd isotope largely vary within the depletion step due to spatial shielding. Thus, the current depletion step such as 2 GWd/t is too coarse to perform the number density calculation only from two-point fluxes and micros, at the beginning and at the end of the depletion step. Accordingly, the method was studied where the number density calculation is performed after the depletion step is divided into several sub-steps for such cases.
The sub-step size was determined to be 0.5 GWd/t, therefore the division into 4 sub-steps is carried out, in the case the local depletion step interval is 2 GWd/t. As shown in Figure 12, the neutron flux, ϕ_{EOS}, and the number density, N_{EOS}, at the end of the coarse step (EOS) are firstly calculated as the predictor part using the neutron flux, ϕ_{BOS}, and the number density, N_{BOS}, at the beginning of the step (BOS). Next, the neutron flux, ϕ_i, per each sub-step can be obtained by interpolating ϕ_{BOS} and ϕ_{EOS}. The number density, N_i, at each sub-step is sequentially obtained from this ϕ_i and from the micro cross-section that corresponds to the end of each sub-step, and N_{EOS} is determined finally. When N_{EOS} is determined, ϕ_{EOS} is updated according to the normal iterative procedure. In other words, this technique is equivalent to performing the corrector part calculation for several sub-steps composing a coarse step instead of the normal corrector part carried out for a single coarse step. Of course, this process is repeated until the convergence of ϕ_{EOS}.

4.2 VALIDATION

Figure 13 shows the results of investigation of the number density change of Gd155 and Gd157 for the typical Gadolinia fuel (Case B1), with the same method as described in Section 3. By

using the sub-step technique, the tracking error of the number density has been reduced without much increasing its running time. Also, Figure 14 shows the error of infinite multiplication factor due to depletion for the same case, and it is concluded that the validity of this method can be confirmed even from the viewpoint of the reactivity.
This method can be utilized for a lot of calculations of the same kind, even for other applications.

5. VALIDATION

The validation for the normal UO_2 fuel and Gadolinia fuel was described in Section 3 and Section 4. Here is described the validity confirmation calculation result for MOX fuel.
Figure 15 and Figure 16 show the errors of the number density tracking calculation of major actinides at 20 GWd/t and those of the infinite multiplication factors due to depletion for Case C1 with the same method described in Section 3. From these figures, it can be confirmed that the calculation with the model discussed in this paper can adequately capture the depletion history also for MOX fuel.
Moreover, Figure 17 shows the comparison of the reactivity loss due to storage before loading between by ANC calculation with the model and by PHOENIX-P reference calculation for the same MOX fuel[5]. This reactivity effect is caused by β decay from Pu241 to Am241 (half life: approximately 14 years), and it can be said that the reactivity effect during the core shutdown or storage period can be adequately expressed.

6. DISCUSSION

In the macro cross-section correction, since the contribution of each nuclide is replaced with the contribution from two group calculation, an error from this point can also be included in the two group macro cross-section reproduced from this method, as well as the number density tracking error. However, judging from the analysis results, it can be said that the calculation accuracy of the number density in this micro-depletion method is considerably good even with the two group calculation and the reactivity effect can be also reasonably incorporated. For the PWR core design, it is considered to be practically enough.
In the case this micro-depletion method is applied to actual core design, designers do not have to calculate a large number of cross-section sets but minimum number of sets for each fuel type. This is because the cross-section set used for the core calculation can be provided without any care for its history. Thus, it is very useful from the viewpoint of efficiency improvement. Furthermore, if a designer wants to account for the as-built enrichment for each fuel region or fuel assembly, he does not have to re-calculate the cross-section sets individually. The micro-depletion model discussed in this paper will be able to capture the initial difference of isotopic contents. Also, this can be expanded to the cross-section sets for recycled uranium fuel containing U234 and U236. Moreover, in future, it will be possible to follow the realistic isotopic weight for every fuel assembly according to the depletion history using this micro-depletion method, instead of the conventional burnup dependent isotope table. Table III shows the difference of the isotope weight in the case where the different depletion history of the typical

PWR fuel is taken into account. The error of the isotopic weight observed here will be considerably reduced if the micro-depletion method is introduced.

CONCLUSION

By introducing the micro-depletion method based on two-group calculation, the prospect that the local depletion history effect can be adequately captured has been obtained, in this research. Also, it was confirmed that reasonable results were obtained, after the investigation of several methods to improve the calculation accuracy, that is, spectral correction model and sub-step technique. In the future, it will be aimed at to improve them further and to investigate the applicability to actual PWR core designs.

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Table I. Survey Cases for Correlation between Micro Cross-section and SIR

Fuel [a]	Case	Condition			Calculation [b]	Remarks
		Relative Power	Boron (ppm)	Moderator Temp. (F)		
$\underline{UO_2}$ ($2.0wt\%U^{235}$) ($4.1wt\%U^{235}$) ($5.0wt\%U^{235}$) $\underline{GAD}$ ($6wt\%Gd_2O_3$) $\underline{MOX}$ ($6.1wt\%Pu^{fis}$) $\underline{BPA}$ (24 PyrexBP)	0	1.0	500	572	Deplete	Base Case
	1	1.5	500	572	Deplete	
	2	0.5	500	572	Deplete	
	3	1.0	500	536	Deplete	
	4	1.0	500	604	Deplete	
	5	1.0	0	572	Deplete	
	6	1.0	1000	572	Deplete	
	7	1.0	2000	572	Deplete	
	8	1.0	0	572	Branch	
	9	1.0	1000	572	Branch	
	10	1.0	2000	572	Branch	

[a]Westinghouse Type Standard 17x17 Fuel Assembly for all case. U^{235} enrichment of 4.1wt% is for GAD and BPA.
[b]Deplete: Depletion Calculation from 0GWd/t to 60GWd/t
Branch: Branch Calculation at Every 10GWd/t on Base Case

Table II. Validation Test Cases

Case	Fuel [a]	Condition			Calculation [b]
		Relative Power	Boron (ppm)	Moderator Temp. (F)	
A0	$UO_2(4.8wt\%U^{235})$	1.0	500	572	Deplete
A1	$UO_2(4.8wt\%U^{235})$	1.0	1000	572	Deplete
A2	$UO_2(4.8wt\%U^{235})$	0.5	500	572	Deplete
B1	$GAD(6wt\%Gd_2O_3)$	1.0	0	572	Deplete
C1	$MOX(6.1wt\% Pu^{fis})$	1.0	1000	572	Deplete

[a]Westinghouse Type Standard 17x17 Fuel Assembly for all case. U^{235} enrichment of 4.8wt% is for GAD.
[b]Deplete: Depletion Calculation from 0GWd/t to 60GWd/t

Table III. Comparison of Isotopic Weight of U235
between Nominal and Off-nominal Power Case
(17x17 Assembly, 4.80wt%U235)

Burnup (GWd/t)	Relative Power = 1.0	Relative Power = 0.5	
	U235 Weight (wt%)	U235 Weight (wt%)	Difference (%)
0	4.80	4.80	0.0
10	3.76	3.75	-0.1
20	2.91	2.89	-0.5
30	2.22	2.19	-1.3
40	1.65	1.61	-2.5
50	1.20	1.15	-4.1
60	0.85	0.79	-6.4

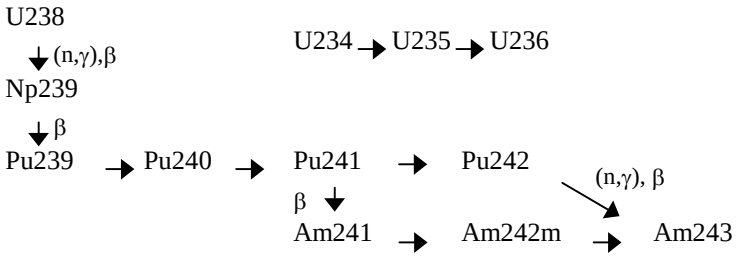

Figure 1. Explicit Tracking Chain (Actinide).

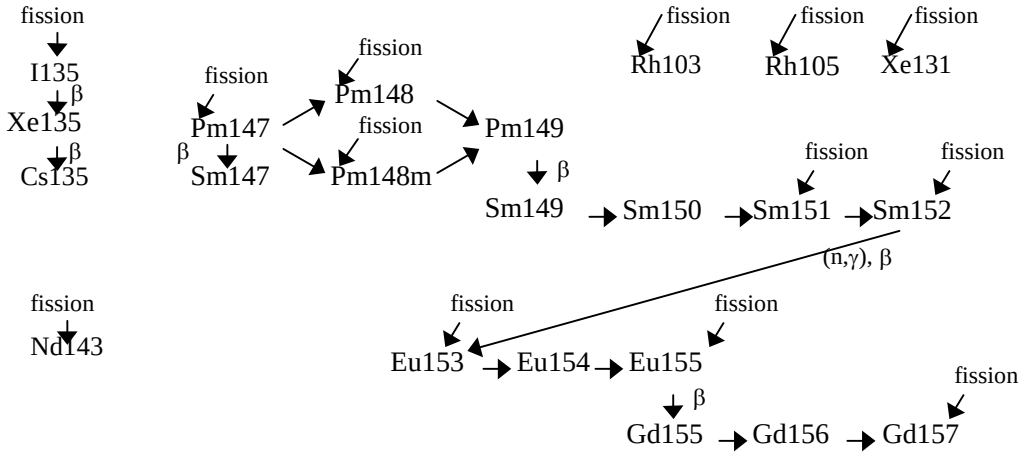

Figure 2. Explicit Tracking Chain (Fission Product).

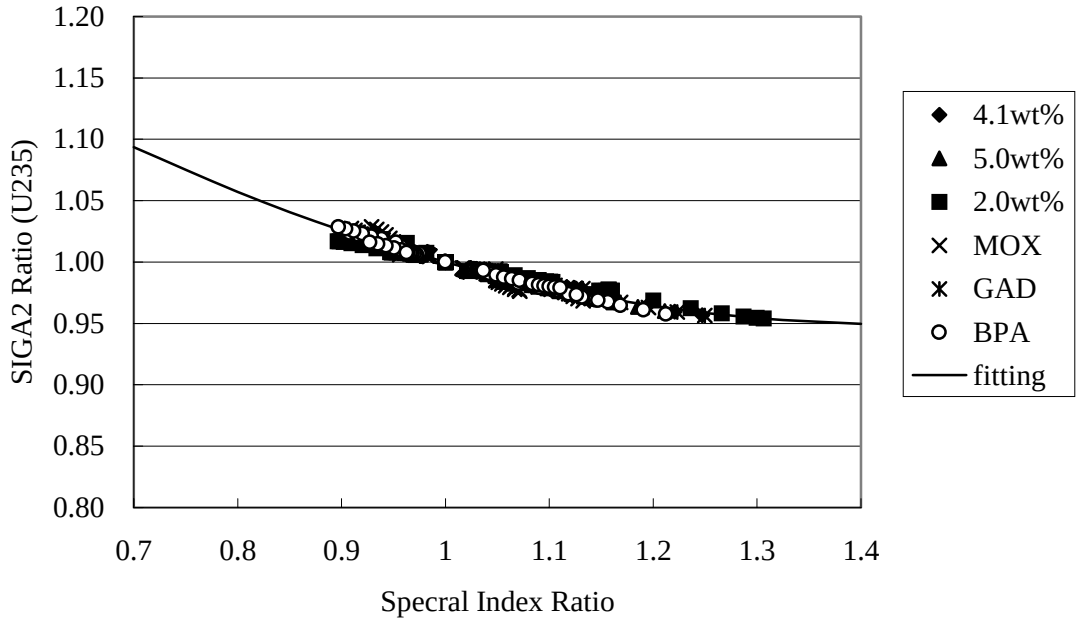

Figure 3. Example of Correlation between Micro Cross-section and Spectral Index Ratio (U235 thermal absorption)

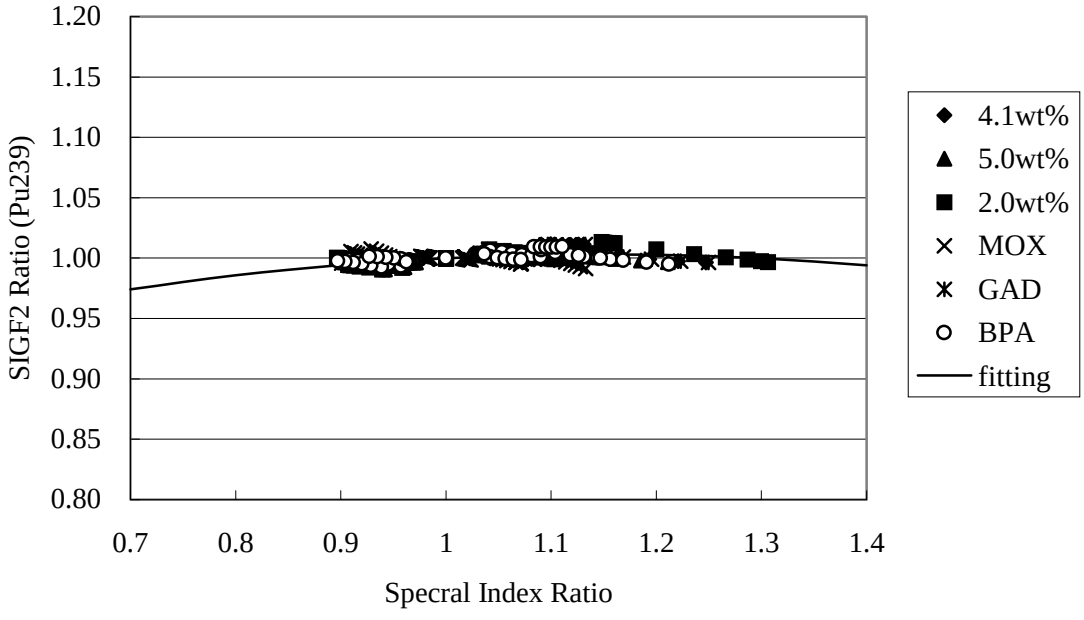

Figure 4. Example of Correlation between Micro Cross-section and Spectral Index Ratio (Pu239 thermal fission)

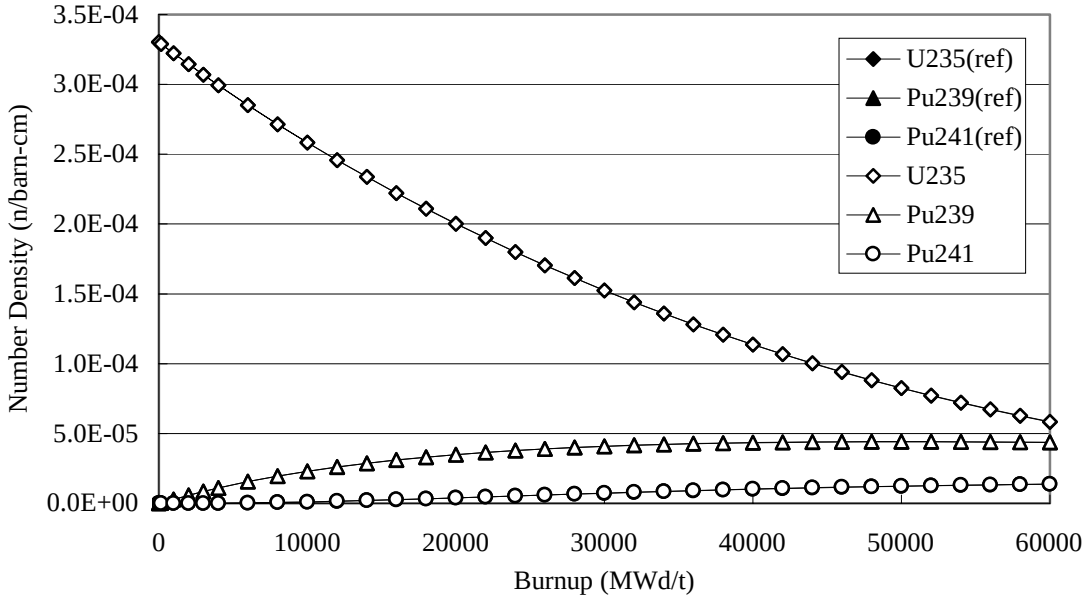

Figure 5. Comparison of Tracked Number Density (Case A0)

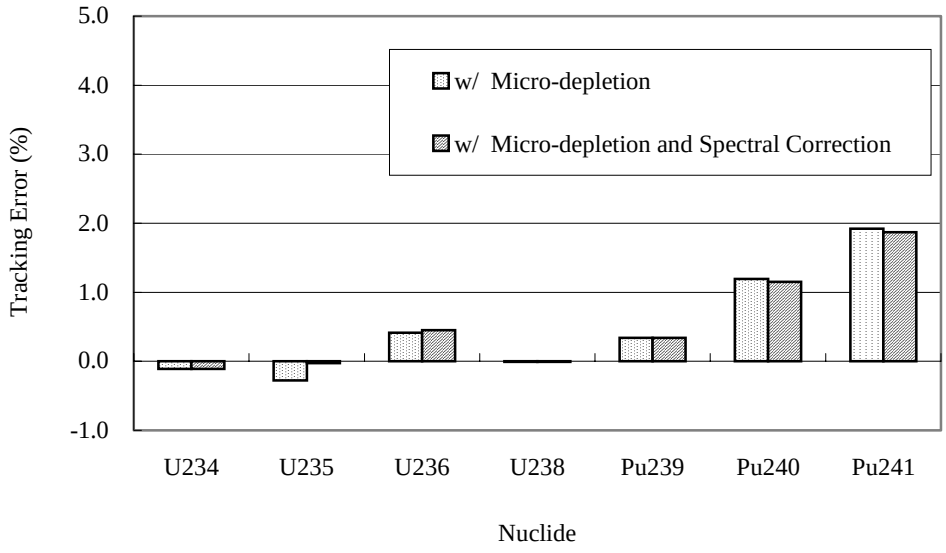

Figure 6. Tracking Error of Number Density at 20GWd/t (Case A0)

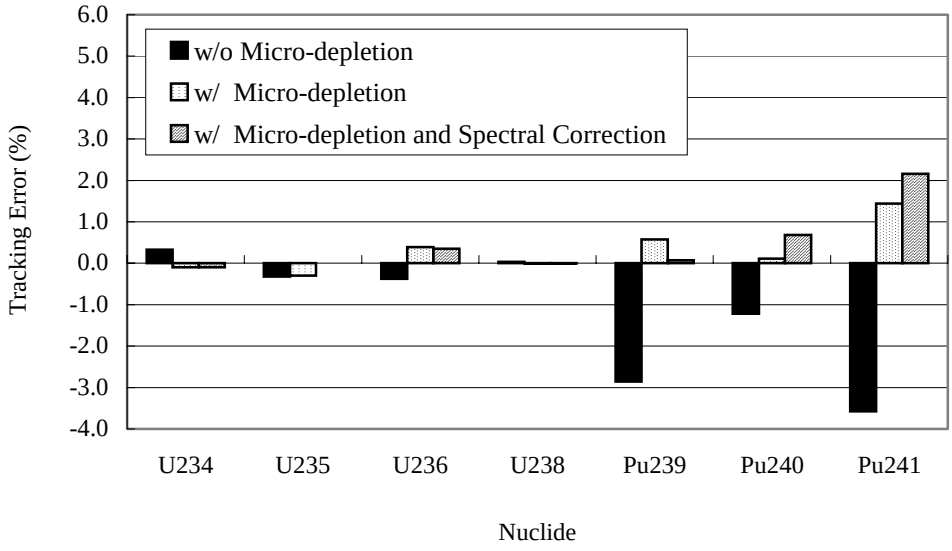

Figure 7. Tracking Error of Number Density at 20GWd/t (Case A1)

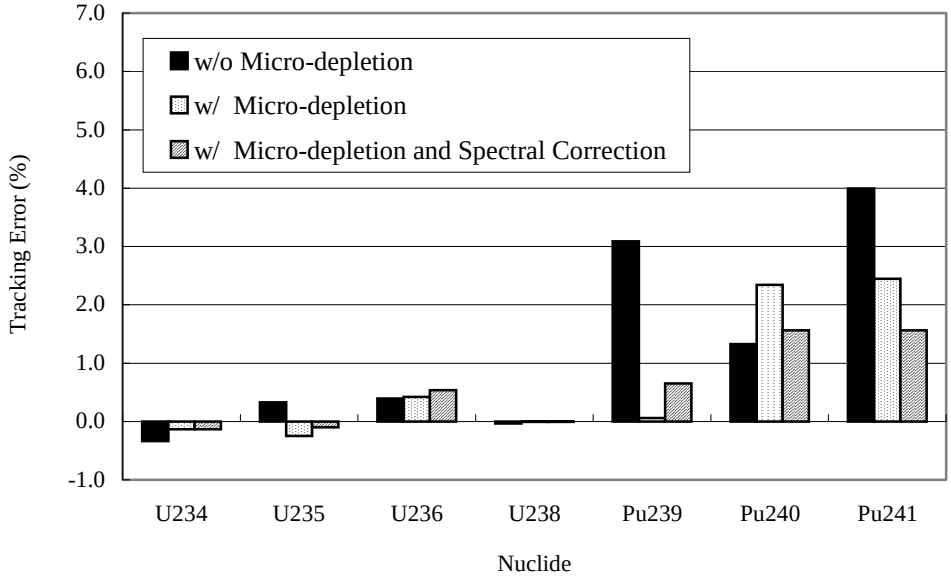

Figure 8. Tracking Error of Number Density at 20GWd/t (Case A2)

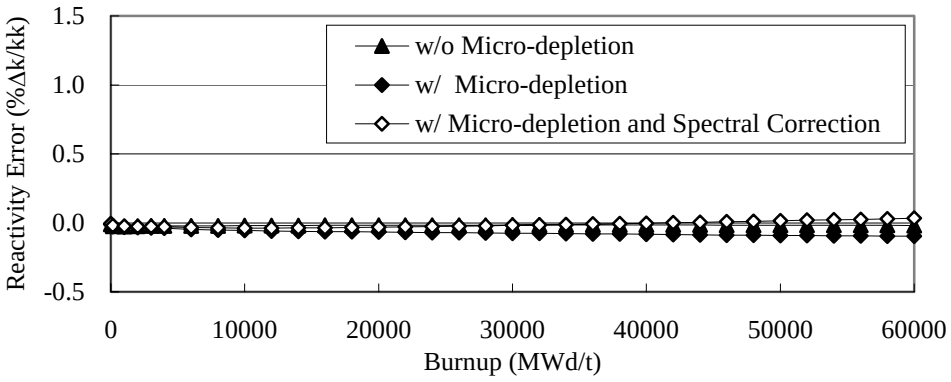

Figure 9. Reactivity Error to Reference (Case A0)

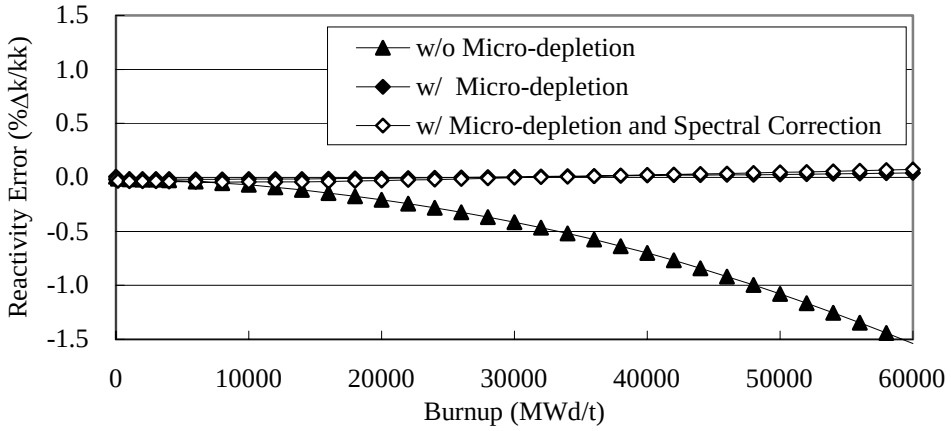

Figure 10. Reactivity Error to Reference (Case A1)

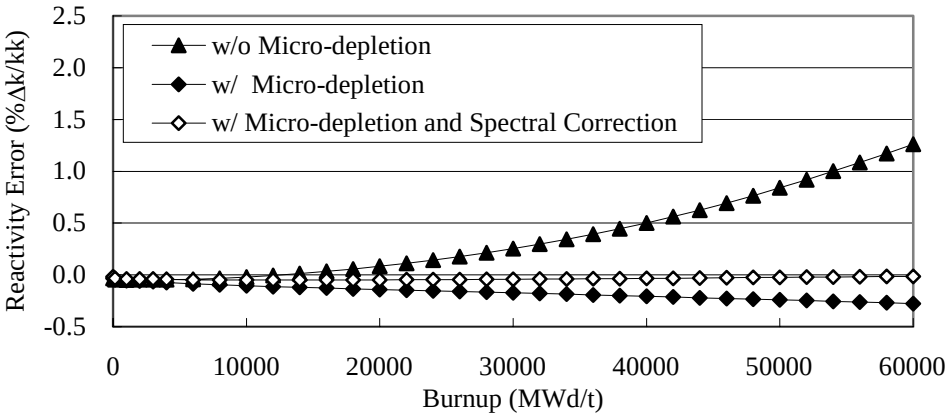

Figure 11. Reactivity Error to Reference (Case A2)

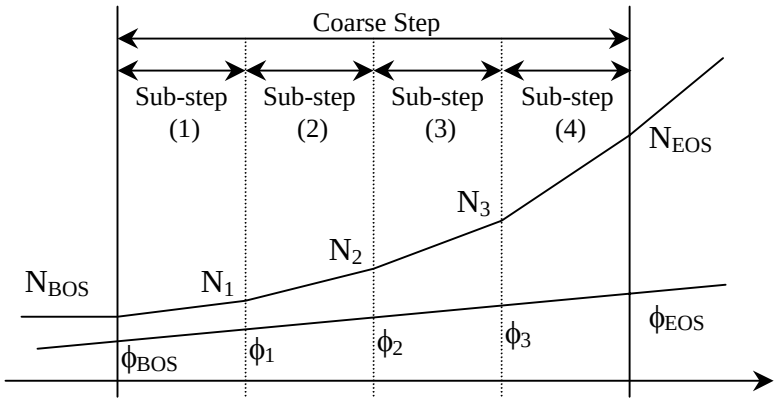

Figure 12. Image of Sub-step Depletion Technique

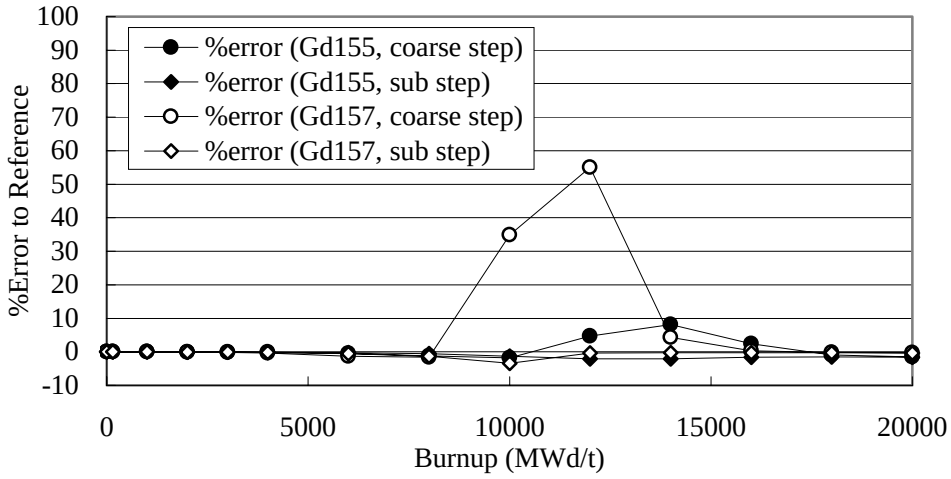

Figure 13. Comparison of Tracked Gd Number Density (Case B1)

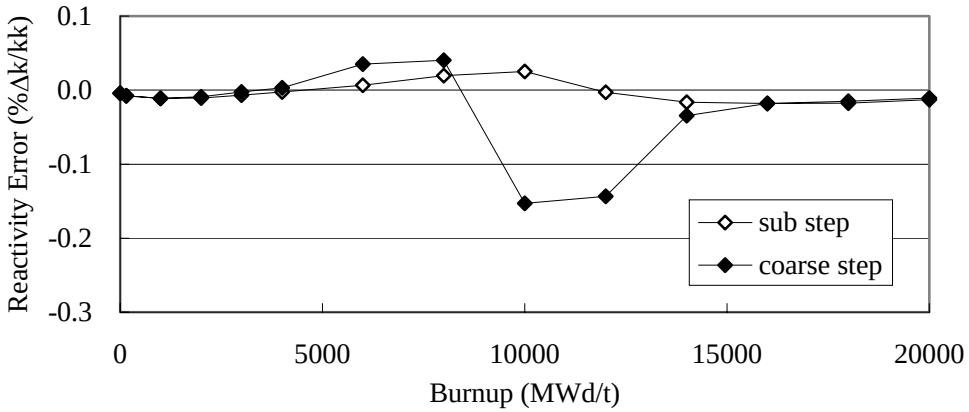

Figure 14. Reactivity Error to Reference (Case B1)

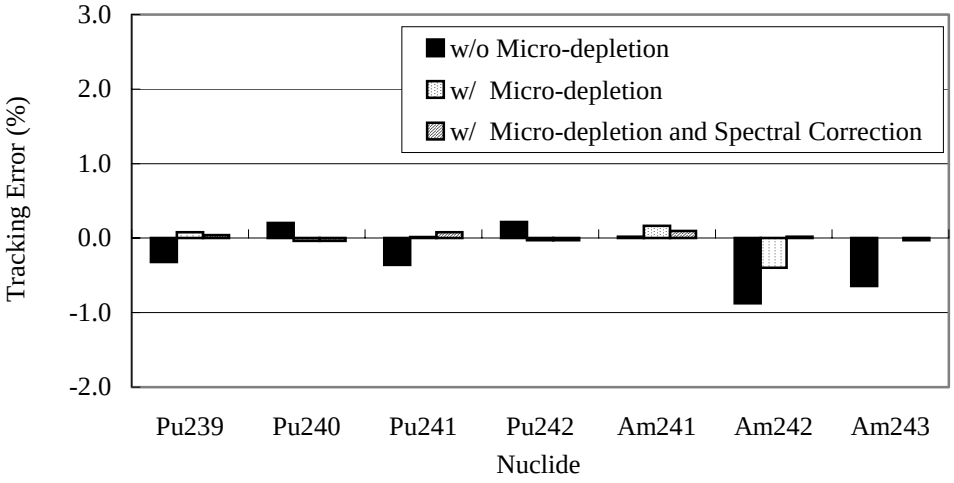

Figure 15. Tracking Error of Number Density at 20GWd/t (Case C1)

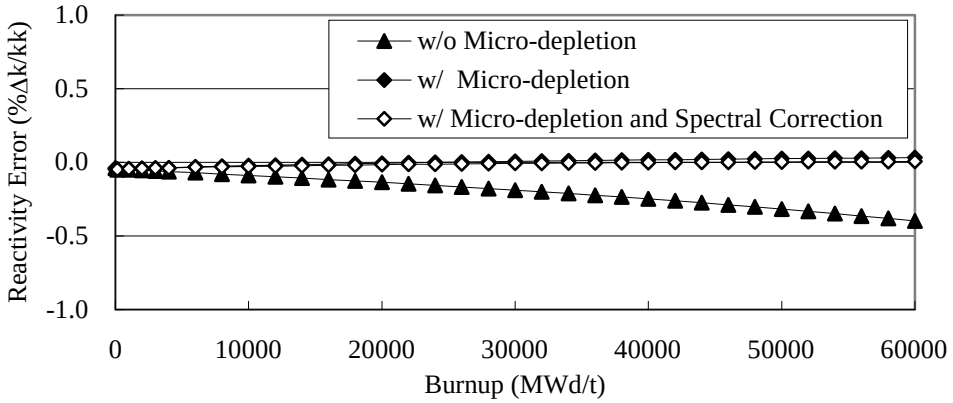

Figure 16. Reactivity Error to Reference (Case C1)

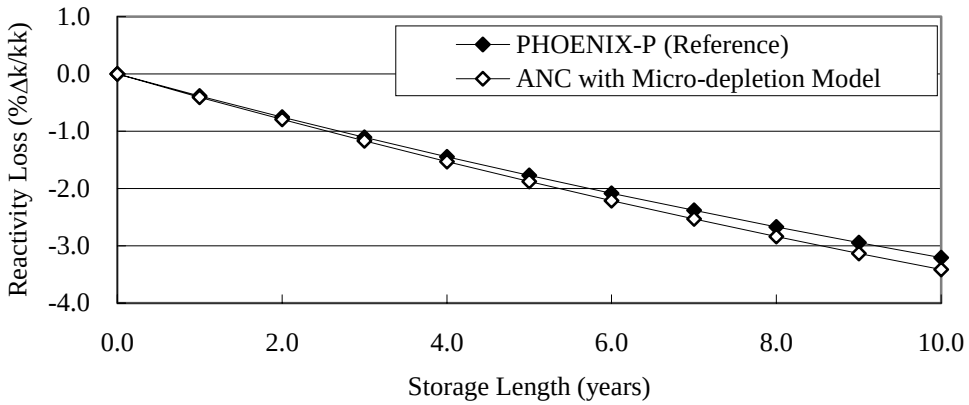

Figure 17. Comparison of Reactivity Loss for MOX fuel due to Storage