# A STUDY ON GENERIC TWO-GROUP CROSS-SECTION REPRESENTATION METHODOLOGY

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## ABSTRACT

Two-group cross-sections are widely used in LWR core design diffusion codes. These two-group cross-sections are generated through assembly calculations at certain reference conditions. Different methods have been used to obtain cross-sections at actual operating conditions based on the reference data. Theoretically, a two-group cross-section is a function of the actual spectrum. This study attempts to find a generic way to capture the features of a spectrum. It is found that the spectrum can be effectively represented by using three spectrum parameters, i.e. the spectrum index (*SI*), the fuel and moderator temperatures ($T_f$ and $T_m$). These three parameters are available in core calculations. Based on this study, a new two-group cross-section representation method is proposed. In the new method, instead of the spectrum, two-group cross-sections are expressed as functions of the spectrum index, moderator and fuel temperature. With the new method, the local cross-sections in a core can be easily derived according to the reference and the actual operating conditions (*SI*, $T_f$, $T_m$). Tests of the new method are performed by calculating cross-sections of unit assemblies at off reference conditions using a diffusion code incorporated with this new method. All results show that the new method can excellently reproduce the cross-sections and the reactivity as compared to the values explicitly calculated by a lattice transport code at the same conditions.

## 1. INTRODUCTION

Most LWR core design diffusion codes use two group cross-sections. The two group cross-sections are generated through assembly calculations by multi-group lattice transport codes at certain reference conditions. For design applications to actual core operating conditions, these constants either have to

be generated with reference conditions very close to the designed core conditions or they have to be generated for a large variety of reference conditions which span over the designed core conditions. The core condition, such as boron letdown curve for each cycle, is unknown before finishing the design. So the former approach requires frequent group constants generation for different core designs, while the latter approach requires a very large tabulation of pre-generated group constants. The matter is further complicated by the fact that the history of the core condition is important as well. It is tempting to come up with a generic and compact representation method to replace the huge tabulation or the frequently repeating group constants generation. Such a representation method can not rely on empirical fit or correlation only, but must be built on some theoretically grounded scheme. This paper discusses the development of such a method, and some preliminary results of using the method.

## 2. DECRIPTION OF THE METHODOLOGY

The proposed representation method addresses both the microscopic cross-section of an isotope and its number density included macroscopic cross-section. While the number density depends on the history of depletion, the microscopic cross-section depends only on the current spectrum and is independent of what history leads to the current spectrum. The key question is how to effectively capture the features of a spectrum. In a two-group diffusion code, the only available spectrum parameters are the Spectrum Index (*SI*, fast to thermal flux ratio), the moderator temperature ($T_m$) and the fuel temperature ($T_f$). They can be calculated during feedback iterations using the information on the core power distribution and the local enthalpy. Past experience shows that using only the spectrum index is not sufficient, giving only partially successful results[1]. Although the spectrum index provides the hardness or softness of a spectrum, the shapes inside the thermal and fast region are characterized respectively by the thermal Maxwellian temperature and the epi-thermal resonance temperature. We therefore propose a generic two-group cross-section representation in terms of the three parameters, *SI*, $T_f$ and $T_m$,

$$\sigma_g = \sigma_g^{ref} \cdot f_g\left(SI, T_f, T_m\right) \qquad g = 1,2 \tag{1}$$

Here $\sigma_g^{ref}$ is the microscopic cross-section at a specified reference condition, and $f_g$ is the spectrum correction factor at any off-reference condition characterized by $\left(SI, T_f, T_m\right)$. For a macroscopic cross-section such as the assembly averaged fuel cross-section, the consistent expression including all isotopes is therefore,

$$\Sigma_g = \sum_i N_i \sigma_g^i = \sum_i N_i \sigma_g^{i,ref} \cdot f_g^i\left(SI, T_f, T_m\right) \tag{2}$$

Unlike microscopic cross-sections, which depend on the current spectrum not the history of the spectrum, number densities depend on the history of the spectrum not the current spectrum. Therefore, for a given fuel composition where the isotopic mixture is specified, the variation of the fuel

macroscopic cross-section versus the current spectrum can be simplified by introducing an "effective" spectrum correction factor as follows,

$$\Sigma_g = \left( \sum_i N_i \sigma_g^{i,ref} \right) \cdot \bar{f}_g \left( SI, T_f, T_m \right) \tag{3}$$

In a typical design code, the fuel macroscopic cross-sections are the only macroscopic cross-sections input to the code; all other input cross-sections are microscopic. The microscopic cross-sections in a design code are used for isotopes whose number densities are explicitly tracked, such as in feedback calculation, burnable absorber depletion, and (fuel exposure history dependent) actinide and fission product micro-depletion correction calculation. Hence if equations (1) and (3) could generically represent the microscopic cross-sections for tracked isotopes and the fuel macroscopic cross-sections, then all the cross-section needs for a design code could be provided. The actual cross-section is determined as:

$$\Sigma_g^{actual} = \left( \sum_i N_i^{ref} \sigma_g^{i,ref} \right) \cdot \bar{f}_g \left( SI, T_f, T_m \right) + \sum_j \sigma_g^j \left( N_j^{actual} - N_j^{ref} \right) \tag{4}$$

Where $N_j^{actual}$ and $N_j^{ref}$ respectively stand for the actual and the reference number density for tracked isotope *j*, and $\sigma_g^j$ is its actual microscopic cross-section calculated using equation (1).

In equation (3), $\bar{f}_g$ depends on the isotopic mixture in the fuel, which is implicitly determined via fuel depletion at a reference condition, e.g. hot full power condition. Any significant deviation from the reference isotopic mixture is accounted by explicitly tracking actinides and fission products for the micro-depletion correction.

As mentioned in the above, the spectrum correction factor $f_g$ is to capture the cross-section variation with the spectrum. It differs from isotope to isotope. The effective spectrum factor $\bar{f}_g$ is defined by weighting $f_g$ over all isotopes in the assembly. The number density dictates the weighting factor for the isotope. For different types of assembly, if their isotope compositions are very similar, especially for the heavy metal isotopes, their effective spectrum factors $\bar{f}_g$ are expected to be almost the same.

Therefore in equation (3), $\bar{f}_g$ should depend mainly on the fuel enrichment and the accumulated burn-up exposure, not on the fuel type except for very different fuel types such as MOX versus $UO_2$ or PWR versus BWR. Our study has confirmed that $\bar{f}_g$ is indeed quite independent of assembly type and smoothly varies with enrichment and burn-up. In other words, the fitting coefficients in $\bar{f}_g\left(SI, T_f, T_m\right)$ turn out to be dependent on the fuel enrichment and burn-up only.

Since the key point of the method is to calculate the spectrum correction factor, we will call it the Spectrum Correction method (SPC).

## 3. SPC MODEL DEVELOPMENT

### 3.1 DATABASE GENERATION AND FITTING

As described in the above, the coefficients in $\bar{f}_g\left(SI, T_f, T_m\right)$ are expected to be dependent on enrichment and burn-up, but almost independent of assembly type. A vast database was therefore generated for various types of PWR assemblies using the Westinghouse lattice transport code ALPHA/PHOENIX-P[2]. The database contains the cross-sections for the fuel types listed in Table I. With different inlet temperature, power level or boron concentration, a total of 28 cases, including 22 hot and 6 cold cases, were covered for each fuel type. In each of the 22 hot cases, the fuel was depleted to 80GWd/t with 26 steps. Branch calculation was applied at each depletion step for the cold cases.

The database contains all the macroscopic cross-sections and the microscopic cross-sections for isotopes that are tracked in the Westinghouse diffusion code ANC[3]. For each cross-section of each isotope, all the data with the same enrichment and the same burn-up are collected for one fit to the function $\bar{f}_g\left(SI, T_f, T_m\right)$. There are 256 such data points in each fit for enrichment of 4.1wt% or 5.0wt%, and 112 data points in each fit for enrichment of 2.1wt%.

Table I. Content of database for cross-section fitting

| Fuel type No. | Specification | Enrichment |
|---|---|---|
| 1 | 14X14 normal | 2.1, 4.1, 5.0wt% $UO_2$ |
| 2 | 14X14 w/ 68Er | 4.1, 5.0wt% $UO_2$ |
| 3 | 15X15 normal | 2.1, 4.1, 5.0wt% $UO_2$ |
| 4 | 15X15 w/ 16Gd | 4.1, 5.0wt% $UO_2$ |
| 5 | 15X15 w/ Pyrex | 4.1, 5.0wt% $UO_2$ |
| 6 | 16X16 normal | 2.1, 4.1, 5.0wt% $UO_2$ |
| 7 | 16X16 w/ 8Gd | 4.1, 5.0wt% $UO_2$ |
| 8 | 17X17 normal | 2.1, 4.1, 5.0wt% $UO_2$ |
| 9 | 17X17 w/ 16Gd | 4.1, 5.0wt% $UO_2$ |
| 10 | 17X17 w/ Pyrex | 4.1, 5.0wt% $UO_2$ |

In this study, the cross-section for hot full power (HFP) with 500ppm boron concentration was used as the reference base case. Figure 1 shows the burn-up dependence of a typical fitting coefficient (in this case for the fit of thermal absorption). The coefficient does change fairly smoothly with burn-up, and so do the other coefficients.

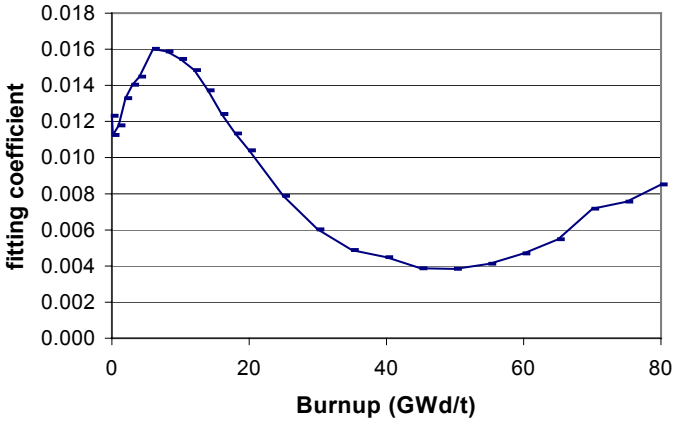


Figure 1. Fitting coefficient change with burn-up for thermal absorption of 4.1wt% $UO_2$

## 3.2 MODEL VERIFICATION

Once the fitting coefficients are given, the actual cross-section can be easily calculated for any given condition using Eq.(4). To check the accuracy of $\Sigma_g^{actual}$, comparison between fit using Eq.(4) and

PHOENIX-P calculation was made for all the macroscopic cross-sections and relevant microscopic cross-sections. As examples, comparisons of macroscopic cross-sections for enrichment of 4.1wt% $UO_2$ are shown in Figure 2 to Figure 7.

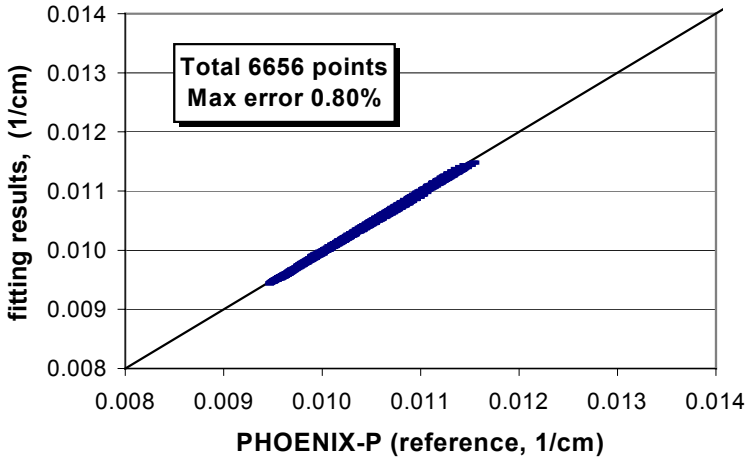


Figure 2. Comparison of fast absorption cross-section fit to PHOENIX-P calculation

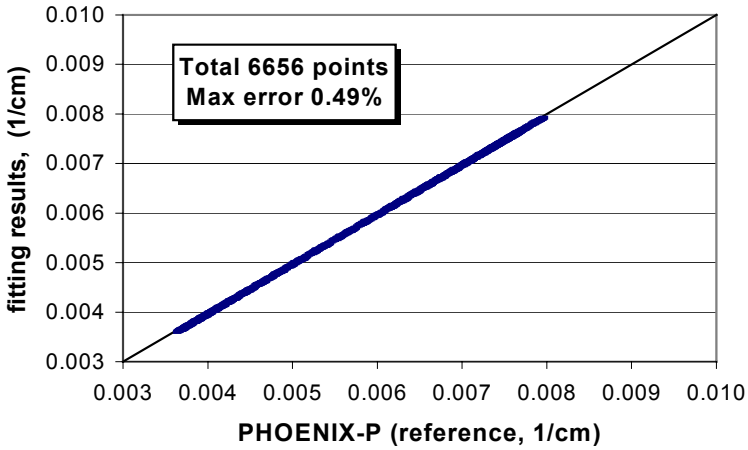


Figure 3. Comparison of fast fission cross-section fit to PHOENIX-P calculation

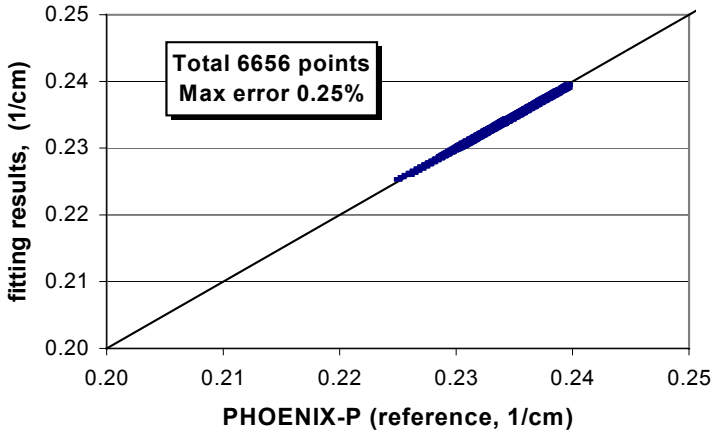


Figure 4. Comparison of fast transport cross-section fit to PHOENIX-P calculation

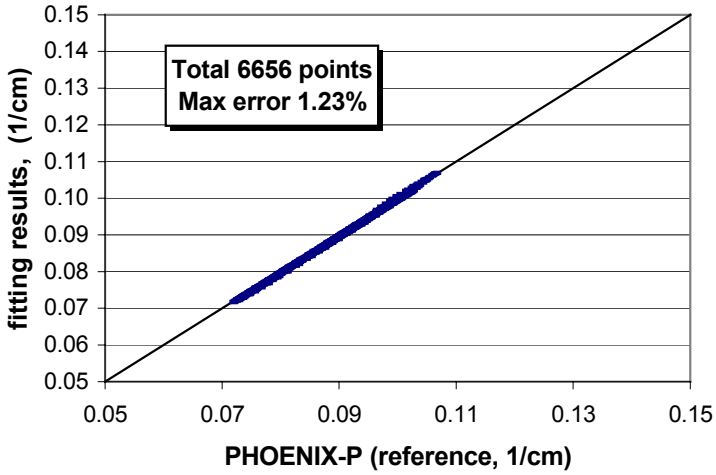


Figure 5. Comparison of thermal absorption cross-section fit to PHOENIX-P calculation

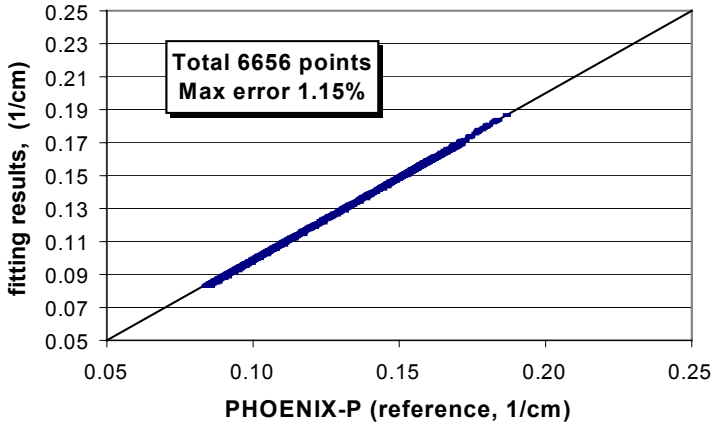


Figure 6. Comparison of thermal fission cross-section fit to PHOENIX-P calculation

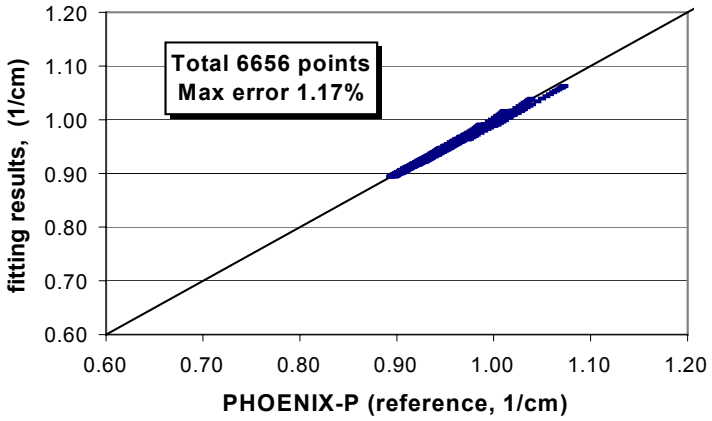


Figure 7. Comparison of thermal transport cross-section fit to PHOENIX-P calculation

At most hot conditions, the cross-section difference between fit and PHOENIX-P calculation is less than 0.5%. At cold condition, the difference goes up to around 1.0% where the actual cross-section variation from the reference base value (HFP) is more than 20%. The comparison shows that this new representation method can capture over 90% of cross-section variation due to spectrum change. Besides, it was found that, in the same energy group, the error of fission cross-section and the error of absorption cross-section are about the same and in the same direction. So the fitting error contribution to reactivity cancels and the accuracy of reactivity should be much better than that of cross-section, as will be seen in the next section.

## 4. BENCHMARK CALCULATIONS

For further evaluation of the new method, ANC was modified to incorporate the method for test problem analysis. Off reference cases for unit assembly (UA) benchmark problems were analyzed for two types of assemblies. These cases are listed in Table II.

Table II. Specification the UA cases

| Case | Assembly | Relative Power (%) | PPM | Remark |
|---|---|---|---|---|
| C1 | 17X17 normal 4.1wt% $UO_2$ | 100 | 500 | Reference base depletion |
| C2 | | 50 | 500 | Off-reference depletion |
| C3 | | 100 | 1000 | Off-reference depletion |
| C4 | | 80 | 1200 | Outside the table depletion |
| C5 | | 0 | 500 | Off-reference cold branch |
| C6 | 16X16 4.16wt% $UO_2$ in average w/ 16Gd | 100 | 500 | Outside the table depletion |
| C7 | | 50 | 500 | Outside the table depletion |
| C8 | | 100 | 1000 | Outside the table depletion |
| C9 | | 50 | 1000 | Outside the table depletion |

It should be emphasized that case C4 is not covered by the database used for calculating the fitting coefficients. Also the 16X16 Gd assembly has different enrichment and number of Gd rods from that listed in Table I. Three-point interpolation in enrichment and burn-up is used in ANC to get the fitting coefficients when they are not provided by the entries of the coefficient table.

ANC input deck was generated by ALPHA/PHOENIX-P at HFP condition with constant boron concentration (500ppm). In the ANC unit assembly model, reflective boundary condition was applied. For the above cases, PHOENIX-P results were provided as the correct solutions to be compared against.

## 4.1 COMPARISON OF REACTIVITY

Figures 8 and 9 show the error of reactivity from ANC as compared to PHOENIX-P for the 17X17 assembly cases and the 16X16 assembly cases, respectively.

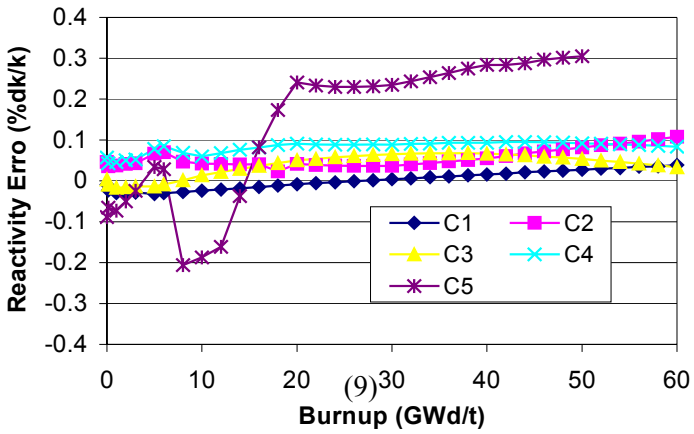

Figure 8. Comparison of $k_\infty$ for the 17X17 $UO_2$ assembly between ANC and PHOENIX-P

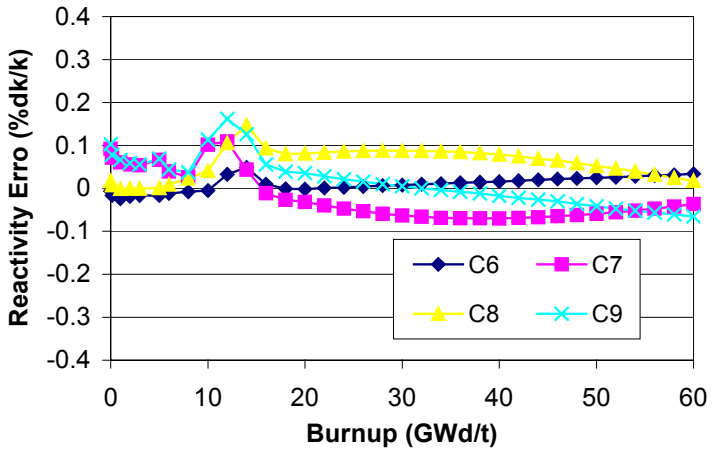


Figure 9. Comparison of $k_\infty$ for the 16X16 $UO_2$/Gd assembly between ANC and PHOENIX-P

Here the reactivity ($k_\infty$) error is defined as:

$$\varepsilon = \frac{\left(k^{anc} - k^{phnx}\right)}{k^{phnx}} \times 100$$

$k^{anc}$ and $k^{phnx}$ are calculated $k_\infty$ by ANC and PHOENIX-P respectively. For all hot condition cases, ANC accurately reproduces PHOENIX-P reactivity even at high burn-up and off-nominal conditions. At cold condition, ANC still works quite well and the maximum difference in $k_\infty$ between ANC and PHOENIX-P is about 0.3% (200~300pcm).

The results of case C4 and all of 16X16 $UO_2$/Gd assembly cases prove that, regardless a condition being covered by the database for coefficient generation, the new cross-section representation method can provide accurate cross-sections for the condition.

To see how big an impact the whole spectrum correction effect can be, test cases C2 and C5 were recalculated by turning off the spectrum correction in ANC (either from the existing method of spectrum correction or the new method of spectrum correction). The comparison of $k_\infty$ is displayed in Figures 10 and 11. It can be seen that the impact of the spectrum correction effect can be very big.

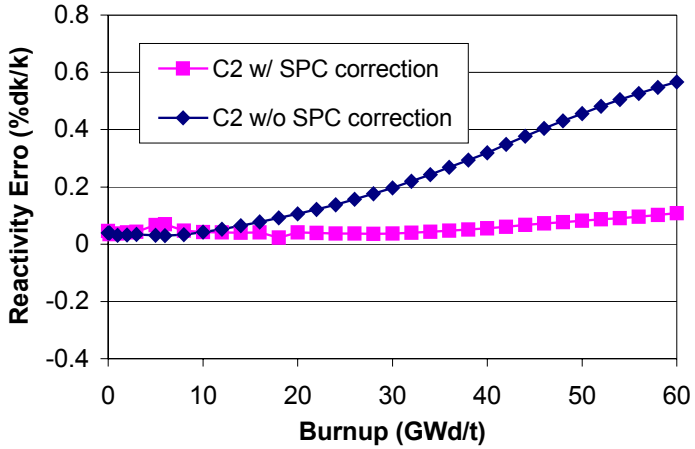


Figure 10. Impact of spectrum correction on reactivity for test case C2(50% power)

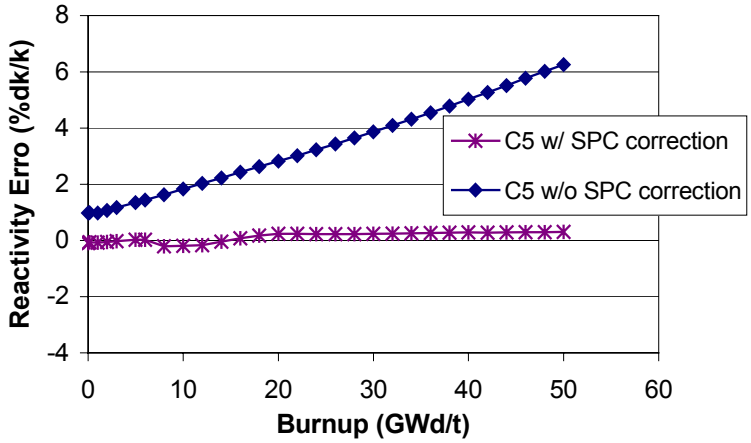


Figure 11. Impact of spectrum correction on reactivity for test case C5(cold case)

## 4.2 COMPARISON OF ISOTHERMAL TEMPERATURE COEFFICIENT

For the two types of unit assembly in Table II, isothermal temperature coefficients (ITC) at hot full power (HFP) and hot zero power (HZP) conditions were calculated for the beginning of cycle case using both PHOENIX-P and ANC. The comparison of ITC given by ANC and PHOENIX-P is shown in Table III. The agreement is very good.

Table III. Comparison of ITC between ANC and PHOENIX-P

| Assembly | | ITC (pcm/°F) | | |
|---|---|---|---|---|
| | | PHOENIX-P | ANC | Delta |
| 17X17 | HFP | -14.6 | -15.7 | -1.1 |
| | HZP | −10.8 | −11.6 | −0.8 |
| 16X16 | HFP | -12.6 | -13.5 | -0.9 |
| | HZP | −10.1 | −10.8 | −0.7 |

## 5. DISCUSSION

Although the results for PWR problem discussed in Section 4 show very good accuracy, there still is room for improvement, especially for cold condition calculation and in ITC calculation. For instance, if the database is not all aggregated as one set but segregated for different fuel types, there is appreciable improvement in the accuracy. Using the function $\bar{f}_g\left(SI, T_f, T_m\right)$ as an interpolation formula for a tabulation in *SI, $T_f$ and $T_m$*, instead of as a representation function should give even higher accuracy.

Due to the much larger spectrum variation associated with the void fraction change in BWR, it is expected to be more challenging to apply the new method of cross-section representation to BWR. A preliminary investigation indicates that the same idea of spectrum correction representation, in terms of $T_f$, $T_m$ and *SI*, works for BWR as well. This is very encouraging. However, the much more complicated heterogeneity of BWR assemblies, in particular the presence of the much different water density in the bypass inside a BWR assembly, requires a careful consideration on the consistency of the method of assembly homogenization and the proposed method of cross-section representation. More work and benchmark calculations are needed and are in progress.

## CONCLUSIONS

A new cross-section representation method, the SPC method, has been developed for diffusion code applications. The method represents the cross-section variation with spectrum in terms of three parameters, the fuel temperature, the moderator temperature and the spectrum index. This new method applies to the full temperature range, from hot operating conditions to the cold shut down condition. Extensive PWR benchmark calculation shows that this generic representation method can accurately

reproduce cross-sections and reactivity of fuel assemblies of many different types and over various conditions. These very encouraging results make it promising that the proposed representation method can be used in lieu of frequent group constants generation or huge cross-section tabulation, which are currently adopted in design codes.

Preliminary investigation on BWR applications shows encouraging results as well, but needs more work to complete. Next phase of the method verification will be on 3-dimensional whole core calculation.

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