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QUALIFICATION TEST OF FEW GROUP CONSTANTS GENERATED FROM AN MC METHOD BY THE TWO-STEP NEUTRONICS ANALYSIS SYSTEM McCARD/MASTER

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ABSTRACT

The purpose of this paper is to examine the qualification of few group constants estimated by the Seoul National University Monte Carlo particle transport analysis code McCARD in terms of core neutronics analyses and thus to validate the McCARD method as a few group constant generator. The two- step core neutronics analyses are conducted for a mini and a realistic PWR by the McCARD/MASTER code system in which McCARD is used as an MC group constant generation code and MASTER as a diffusion core analysis code. The two-step calculations for the effective multiplication factors and assembly power distributions of the two PWR cores by McCARD/MASTER are compared with the reference McCARD calculations. By showing excellent agreements between McCARD/MASTER and the reference MC core neutronics analyses for the two PWRs, it is concluded that the MC method implemented in McCARD can generate few group constants which are well qualified for high-accuracy two-step core neutronics calculations.

Key Words: two- step core neutronics analysis, McCARD/MASTER code system, few group constant generator

1. INTRODUCTION

The two-step procedure is the most common basis of the current neutronics design computations of nuclear reactors. In this procedure, a deterministic assembly or lattice physics code is normally used to determine a multi-group flux distribution in the assembly for generation of homogenized few-group cross sections (few group constants for short hereafter). However, generation of few-group constants in various nuclear applications by the deterministic lattice physics codes has posed many difficulties, which may stem from inherent drawbacks of deterministic methods such as multi-group approximation and inability to describe the detailed geometrical information of the lattices as designed. In very high temperature gas-cooled reactor (VHTR) analysis, for example, there arise accuracy issues concerning the resonance treatment or the double heterogeneity (DH) treatment. As a matter of fact, most of existing transport lattice codes cannot handle the DH problem directly. In some studies, an approximation method called the reactivity-equivalent physical transformation (RPT) [1] was adopted.

As a way to get around the inherent difficulties of deterministic methods and thus to mitigate the accuracy issues, we recently proposed a Monte Carlo (MC) method augmented by the B_1 spectral approximation [2] as an alternative to deterministic methods for few-group constant generation

[3]. The MC method makes the most of its ability to use continuous energy nuclear data and detailed geometric information to simulate the reaction rates with high accuracy. The B_1 spectral approximation not only allows one to take into account the effect of critical spectrum on the fuel depletion and generation of few group constants but also enables one to determine the diffusion constants which are needed for diffusion theory core calculations. We have implemented the proposed MC method into the few-group constant generator module of Seoul National University MC code McCARD, and demonstrated that few group constants generated from McCARD compare very well with those from deterministic lattice physics code HELIOS [4] for a checkerboard FA system of a PWR [5]. The purpose of this paper is to assess the qualification of few group constants from the MC method in terms of the core depletion analysis for a PWR based on a two-step code system McCARD/MASTER in which McCARD is used as an MC group constant generation code and MASTER [6] as a diffusion core analysis code. In so doing we will examine how well core depletion calculations by the two-step McCARD/MASTER code system agree with those by the single step McCARD. We also investigate how significant the effect of the critical spectrum is on generation of few group constants and predictions of the core design parameters with burnup including the k-effective and fuel assembly (FA) power distribution.

2. TWO-STEP CALCULATIONS BY MONTE CARLO METHODS

2.1. Generation of Few Group Constants

The proposed MC method for generation of few group constants is described in detail in references 3 and 5. The following is a brief summary on the method at the risk of repetition. Like its deterministic counterpart, the MC method calls for the solution to the B_1 equation [7];

$$\begin{aligned} \Sigma_{tg}\phi_g \mp BJ_g &= \sum_{g'} \Sigma^{(0)}_{g'g}\phi_{g'} + \chi_g \\ \pm B\phi_g + 3\alpha_g(B)\Sigma_{tg}J_g &= 3\sum_{g'} \Sigma^{(1)}_{g'g}J_{g'} \end{aligned} \tag{1}$$

The notations are standard [7]. Σ_{xg} is the fine-group macroscopic cross sections of the reaction type x defined by

$$\Sigma_{x,g} = \frac{\int_V \int_{\Delta E_g} \int_{4\pi} \Sigma_x(\mathbf{r},E)\phi(\mathbf{r},E,\mathbf{\Omega})d\mathbf{\Omega}dEd\mathbf{r}}{\int_V \int_{\Delta E_g} \int_{4\pi} \phi(\mathbf{r},E,\mathbf{\Omega})d\mathbf{\Omega}dEd\mathbf{r}} \tag{2a}$$

The numerator and the denominator in Eq. (2a) denote the x-type reaction rate, and the neutron flux, of group g neutrons in the volume V, respectively. They can be computed using either track length or collision estimator of MC codes. $\Sigma^{(n)}_{g'g}$ (n=0,1) is the n^{th} Legendre component of group-to-group scattering cross section defined by

$$\Sigma_{g'g}^{n} = \frac{\int_V \int_{\Delta E_g} \int_{\Delta E_{g'}} \Sigma_s^n(\mathbf{r}, E' \to E)\phi^n(\mathbf{r}, E')dE'dEd\mathbf{r}}{\int_V \int_{\Delta E_{g'}} \phi^n(\mathbf{r}, E)dEd\mathbf{r}}; \; n=0,1. \tag{2b}$$

$\Sigma_s^n(\mathbf{r}, E' \to E)$ and $\phi^n(\mathbf{r}, E)$ are the n^{th} Legendre components of the double differential scattering cross-section and the angular flux, respectively. We find it very difficult and prohibitively time-consuming to compute $\phi^1(\mathbf{r}, E)$ as accurate as $\phi^0(\mathbf{r}, E)$ by an MC code. For the computation of $\Sigma_{g'g}^1$ in practice, therefore, we introduced an assumption that $\phi^1(\mathbf{r}, E)$ is proportional to $\phi^0(\mathbf{r}, E)$, which holds approximately good for near-isotropic systems [5]. This assumption is equivalent to computing $\Sigma_{g'g}^{(n)}$ (n=0,1) by

$$\Sigma_{g'g}^{n} = \frac{\int_V \int_{\Delta E_g} \int_{\Delta E_{g'}} \Sigma_s^n(\mathbf{r}, E' \to E)\phi(\mathbf{r}, E')dE'dEd\mathbf{r}}{\int_V \int_{\Delta E_{g'}} \phi(\mathbf{r}, E)dEd\mathbf{r}}; \; n=0,1. \tag{3}$$

Equation (3) suggests that $\Sigma_{g'g}^{(n)}$ (n=0,1) can also be calculated in the same way as Σ_{xg} by any MC codes.

The B_1 solution results in a fine-group critical spectrum, ϕ_g^B, from which one can generate the type x few-group reaction cross sections by

$$\Sigma_{x,G} = \frac{\sum_{g \in G} \Sigma_{x,g} \phi_g^B}{\sum_{g \in G} \phi_g^B} \tag{4}$$

and the few group diffusion constants by

$$D_G = \frac{\pm \sum_{g \in G} iJ_g}{\sum_{g \in G} B_1 \phi_g} \tag{5}$$

2.2. Depletion calculation with critical spectrum

The few group constants with FA burnup can be generated in the same way as above. Because of the fuel depletion and production of new isotopes, however, the number densities of the constituent nuclides must be updated by solving the following the Bateman equations,

$$\frac{dN_{m,i}(t)}{dt} = \sum_j l_{ij}\lambda_j N_{m,j}(t) + \sum_j r_{m,ij} N_{m,j}(t) - (\lambda_i + r_{m,i}^n) N_{m,i}(t); \; t \in [t_n, t_{n+1}] \tag{6}$$

for each nuclide in each region at each depletion time step (DTS). $N_{m,\ell}(t)$ $(\ell = i, j)$ is the number density of nuclide ℓ in cell *m* at depletion time *t*. $r_{m,ij}$ is the fraction of the microscopic absorption reaction rate of nuclide *j* in cell *m* which leads to the creation of nuclide *i*. $r_{m,i}$ is the microscopic absorption rate of nuclide *i* in cell *m*. Other notations are standard. The solution to Eq. (6) requires determining $r_{m,ij}$ and $r_{m,i}$ every beginning of the given DTS by the MC eigenvalue calculation for the given FA. Because $r_{m,ij}$ and $r_{m,i}$ from the MC calculation are based on the infinite medium spectrum, however, they need be corrected in terms of the real core spectrum on fuel depletion. As in the same way as the above, the corrections are made with the critical spectrum that can be obtained by solving B_1 equations at each beginning of the DTS. Actually, we can determine the critical-spectrum-corrected $r^B_{m,ij}$ and $r^B_{m,i}$ by using the group-wise ratio of the assembly-wise critical spectrum (ϕ^B_g) to the infinite medium spectrum (ϕ_g), ϕ^B_g / ϕ_g, as follows;

$$r^B_{m,i} = \sum_g \frac{\phi^B_g}{\phi_g} r^g_{m,i} \quad \text{and} \quad r^B_{m,ij} = \sum_g \frac{\phi^B_g}{\phi_g} r^g_{m,ij} \tag{7}$$

The Bateman equations of Eq. (6) with $r^B_{m,ij}$ and $r^B_{m,i}$ substituted for $r_{m,ij}$ and $r_{m,i}$ are then for each region to determine the new material composition at the end of the DTS or the beginning of the next DTS.

2.3. The McCARD/MASTER code system

In order to examine the qualification of the few group constants generated by the MC method, we combined MASTER [6], a three-dimensional (3-D) core neutronics code, with the few-group cross section generation capability of McCARD to form the McCARD/MASTER code system for two-step core neutronics calculations. The assembly-homogenized few-group constants including diffusion coefficients and pin power form functions are generated by McCARD. As in the conventional two-step procedure, the few-group constants are tabularized as a function of state parameters such as burnup, boron concentration, fuel and moderator temperatures, etc. To automate the repetitive restart calculations for each condition determined by the state parameters, MIG (McCARD Input Generator) and MOCHA (McCARD Output Convertor into HOPE ASCII table) utilities are developed. The two special utilities are used to generate the cross section library and form function files which are needed for the core neutronics calculations by the MASTER code. Figure 2 presents a computational flow chart of the McCARD/MASTER code system.

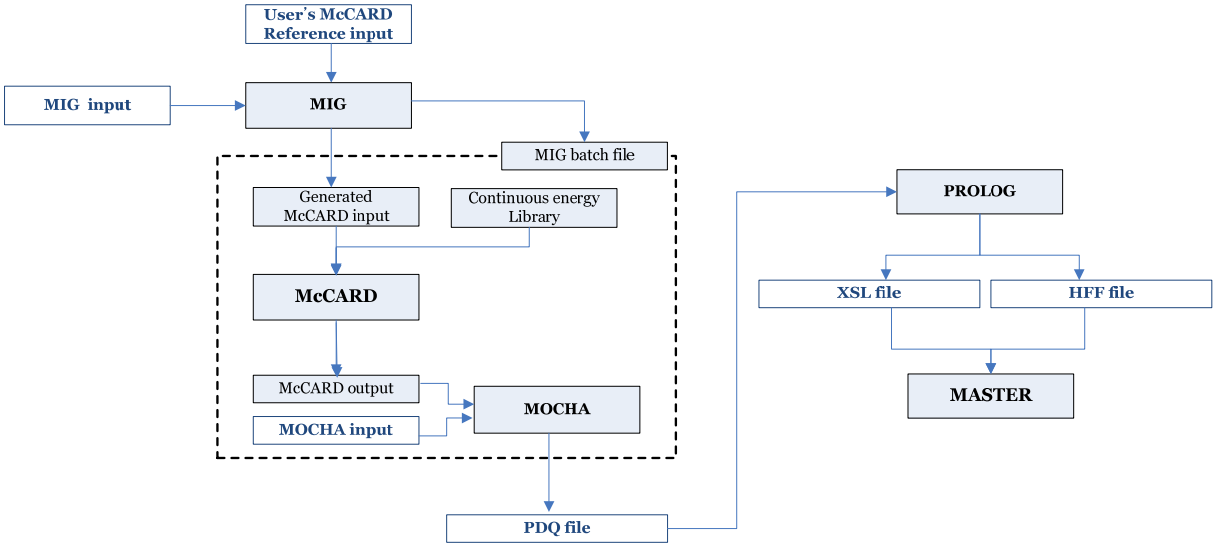

Figure 1. Flow chart of McCARD/MASTER code system

3. APPLICATION FOR PWR CORE ANALYSIS

To examine the qualification of McCARD-generated few group constants, a depletion analysis for a mini-PWR core and its constituent fuel assemblies (FAs) is performed using the McCARD/MASTER code system. The reference solution for the mini-PWR core is obtained from the direct McCARD run based on 1,000 active cycles with 10,000 histories per cycle. The few group constants of FAs needed for core calculations are generated by McCARD based on 200 active cycles with 10,000 histories per cycle at each DTS. The continuous energy cross section inputs to McCARD are taken from ENDF/B-VI.8. The 47-group structure of HELIOS is adopted for generation of the fine group constants and the subsequent B_1 calculations. The power density for MC depletion analysis is set at 20.643 W/gU.

3.1. Single fuel assembly depletion

Figure 2 shows the configuration of three types of 17x17 FAs comprising the mini-PWR core. All the FAs contain 28 guide tubes filled with water in common. The type D0 is unshimmed FA consisting of 264 4.30% enriched UO_2 fuel pins, while the types D1 and D2 shimmed FAs consisting of 248 UO_2 fuel pins plus 16 gadolinia burnable poison rods and 240 UO_2 fuel pins plus 24 gadolinia burnable poison rods, respectively.

Figure 3 shows a comparison of the McCARD and McCARD/MASTER calculations for the burnup-dependent k-infinity of the type D0 FA over burn-up range from 0 to 10 MWd/kgU . The standard deviation of the McCARD depletion runs is in the range of 50~70 pcm. The two calculations agree well with each other within 165 pcm, and the root-mean-square (RMS) difference between k-infinities of the two calculations is observed to be 68 pcm. Figures 4 and 5 compare the McCARD and McCARD/MASTER calculations for the burnup-dependent k-

infinity of the type D1 and the type D2 FA, respectively. The good agreements between the two calculations are also noted in the two shimmed FA types. The RMS difference between k-infinities of the two calculations is 120 pcm for the type D1 FA while it is 165 pcm for the type D_2 FA.

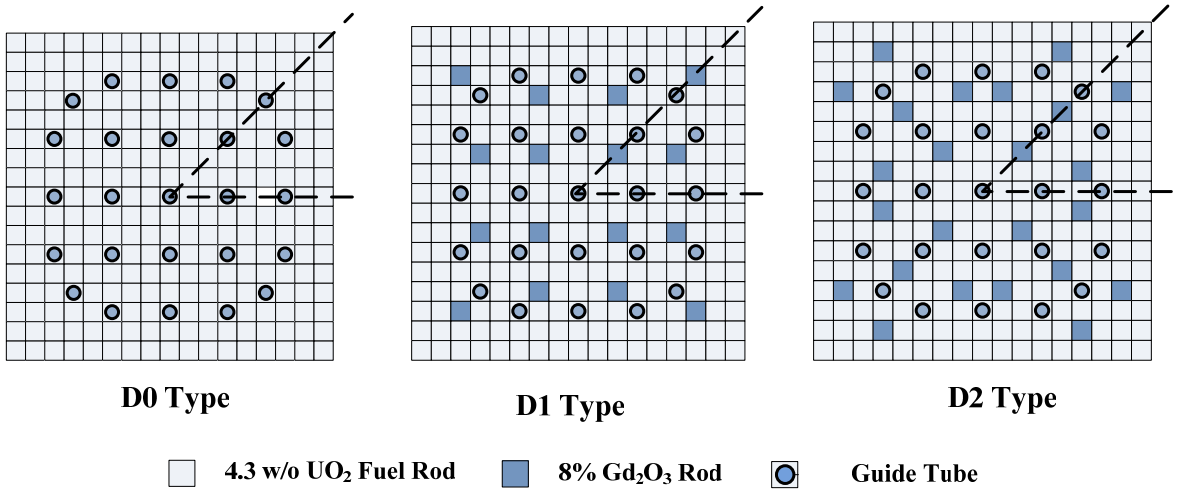

Figure 2. The configuration of three types of PWR fuel assemblies

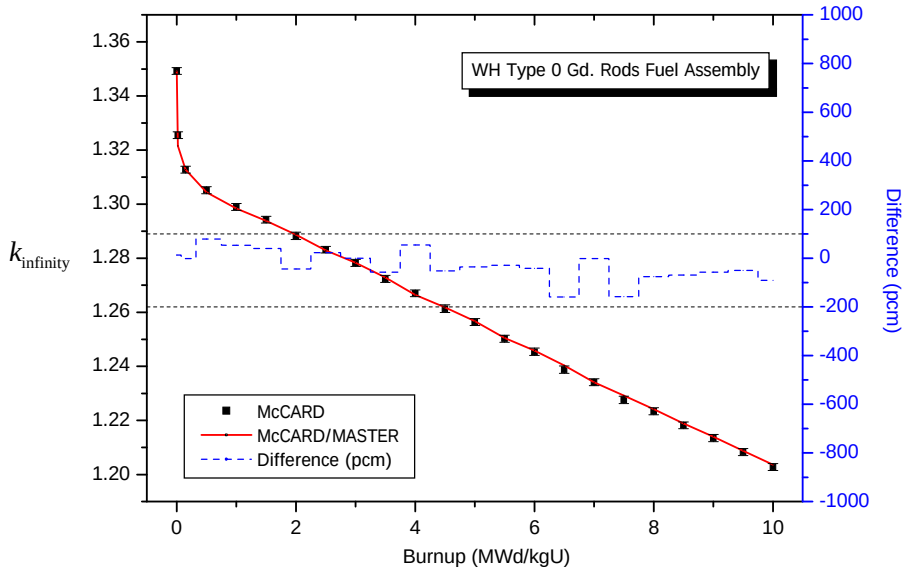

Figure 3. The k-infinity versus burnup for the type D_0 FA

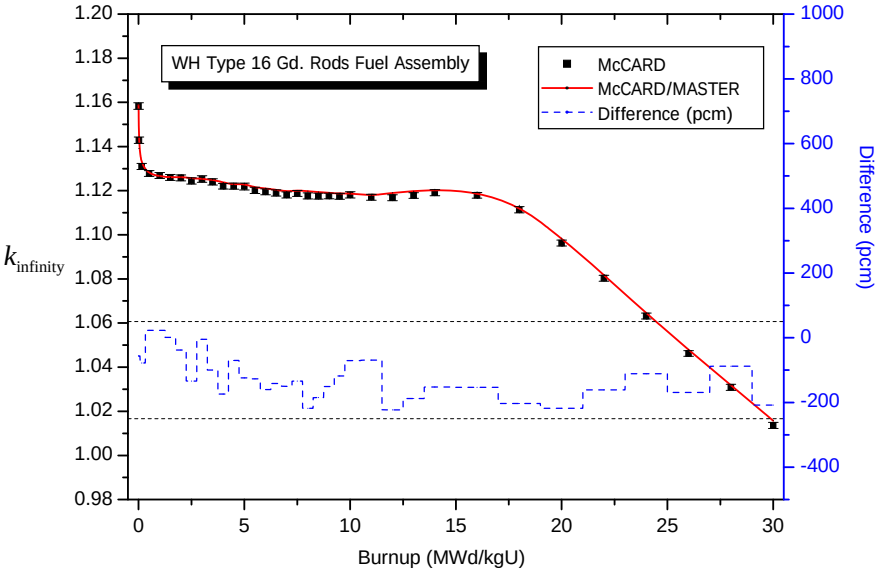

Figure 4. The k-infinity versus burnup for the type D_1 FA

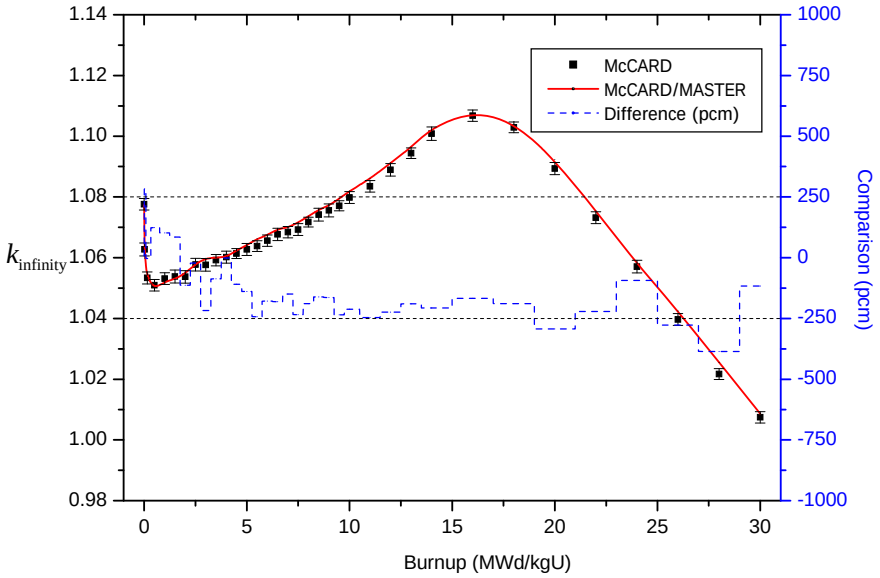

Figure 5. The k-infinity versus burnup for the type D_2 FA

3.2. Two-dimensional (2D) mini-core depletion

Figure 6 shows the configuration of 2D mini-PWR core consisting of the three FA types; D0, D1, and D2 shown above. As mentioned, this problem is designed to examine the qualification of the

few group constants from McCARD and the effect of the critical spectrum on them as well. To examine the latter the two sets of few group constants are produced; one with the use of the infinite medium spectrum and another with the use of the critical spectrum. The two sets are used for predictions of the critical boron concentrations and the assembly-wise power distribution and results of the two predictions are compared in Figs. 7 and 8. The few group constants from the use of infinite medium spectrum result in the RMS error of 49 ppm, while those from the use of critical spectrum 29 ppm, in the critical boron concentration over the core burnup range from 0 to 10 MWd/kgU. The former results in the RMS errors of 1.13% and 1.2%, while the latter 0.53% and 0.87%, in normalized assembly-wise power distributions at 0 and 10 MWd/kgU, respectively. These results clearly indicate that the effect of the critical spectrum on the generation of the few group cross sections is significant in terms of accuracy of the steady-state neutronics analysis by the two-step deterministic approaches.

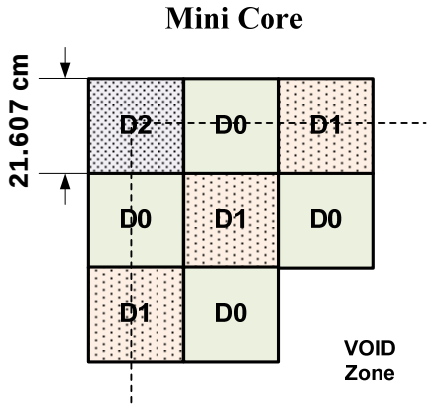

Figure 6. The configuration of PWR 2D mini-core problem

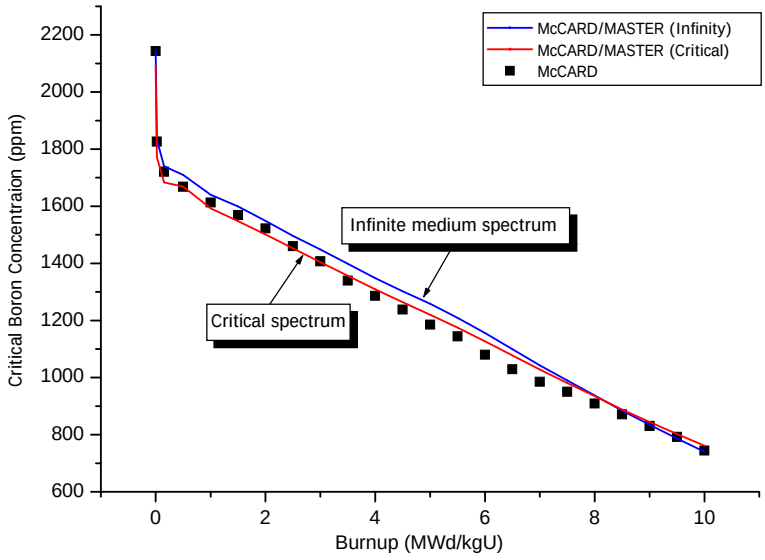

Figure 7. The critical boron concentration for PWR 2D mini-core problem

0MWd/kgU

D_2	D_0	D_1
1.785	1.881	0.684
0.13	0.10	0.16
1.3	-0.9	1.2
-0.7	1.3	-0.7
D_0	D_1	D_0
1.882	1.229	0.504
0.10	0.08	0.14
-0.9	0.6	-0.6
0.4	-0.6	0.4
D_1	D_0	
0.686	0.504	
0.16	0.14	
1.5	-0.7	
0.2	0.3	

1.0 MWd/kgU

D_2	D_0	D_1
1.760	1.838	0.701
0.13	0.10	0.15
0.4	-1.3	1.8
-1.3	0.4	-1.3
D_0	D_1	D_0
1.837	1.236	0.517
0.10	0.08	0.13
-1.3	0.6	-0.1
-0.4	-0.3	0.9
D_1	D_0	
0.701	0.519	
0.15	0.13	
1.9	0.4	
0.7	1.3	

Assembly type
Power of McCARD
Rel. Err. (%)
Diff. (INF)*
Diff. (CRI)**

* Diff(Inf) = (Power by Infinite medium spectrum - Reference)/Reference

** Diff(Cri) = (Power by Critical spectrum - Reference)/Reference

Figure 8. The assembly-wise power distribution for PWR 2D mini-core problem

3.3. A Three-Dimensional Core analysis

For a further examination on the performance of the McCARD/MASTER two-step analysis, a quarter core analysis is made for a more realistic three-dimensional (3D) PWR core consisting of 57 FAs. Figure 9 displays a quarter of the PWR core. Table I shows the effective multiplication factors (k-effective) that are obtained from McCARD/MASTER calculations using two sets of few group constants; one from the use of the infinite medium spectrum and another from the use of the critical spectrum, in comparison with the reference MC calculation by McCARD. The k-effective from McCARD/MASTER based on the critical spectrum agrees very well with, while the k-effective from the use of the infinite medium spectrum is far off, the reference MC result. Figures 10 and 11 show the two McCARD/MASTER calculations for assembly-wise power distribution and the average axial power distribution, respectively, in comparison with the reference MC calculations by McCARD. It is noted that the few group cross section set from the use of the critical spectrum result in much less RMS error than that from the use of infinite medium spectrum in McCARD/MASTER calculations for assembly-wise power distribution. The two few group cross section sets appear to predict the average axial power distribution very similarly. In terms of the RMS error, however, it is noted that the average axial power distribution from the few group cross section set based on the critical spectrum is slightly better than that based on infinite medium spectrum.

Table I. The k-effective for PWR 3D core problem

Case	K-effective	Difference (pcm)
McCARD	1.02907±0.00016	-
McCARD/MASTER (Critical spectrum)	1.02915	8
McCARD/MASTER (Infinite-Medium spectrum)	1.03240	333

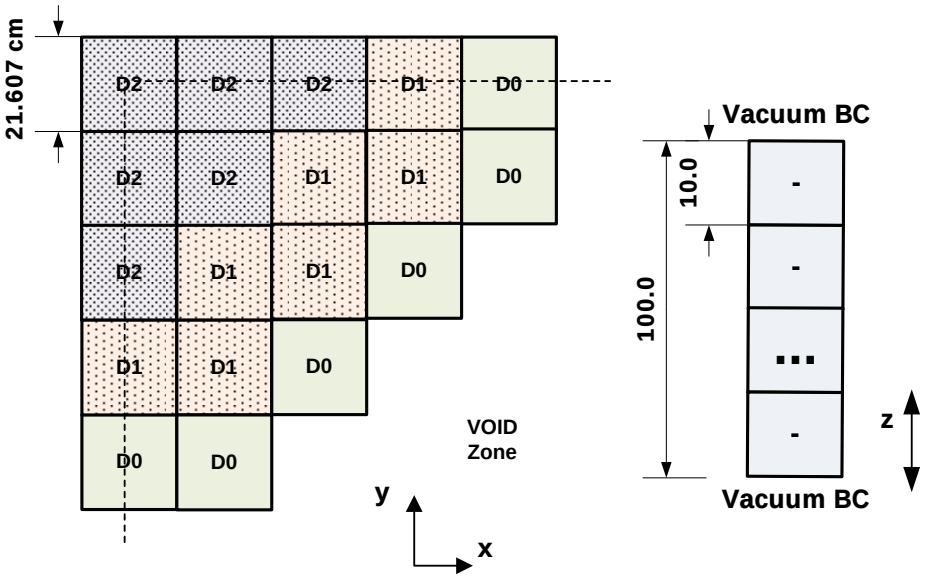

Figure 9. The configuration of PWR 3D core problem

D_2	D_2	D_2	D_1	D_1
1.355	1.366	1.347	1.173	0.527
0.18	0.13	0.13	0.14	0.21
3.72	3.00	1.89	0.10	-1.13
-1.58	-1.54	-0.78	0.78	1.54
D_2	D_2	D_1	D_1	D_0
1.370	1.390	1.431	1.028	0.429
0.13	0.09	0.09	0.11	0.18
2.97	2.34	0.26	-1.19	-4.29
-1.56	-1.33	-0.37	0.37	1.84
D_2	D_1	D_1	D_0	
1.346	1.429	1.150	0.596	
0.13	0.09	0.10	0.15	
2.09	0.57	-1.21	-4.57	
-0.57	-0.06	0.01	0.97	
D_1	D_1	D_0		
1.168	1.025	0.599		
0.14	0.11	0.15		
0.19	-0.77	-4.86		
0.87	0.78	0.69		
D_1	D_0			
0.523	0.424			
0.22	0.18			
-0.51	-3.26			
2.15	2.81			

Assembly type
Power of McCARD
Rel. Err. (%)
Diff. (INF)*
Diff. (CRI)**

* Diff(Inf) = (Power by Infinite medium spectrum - Reference)/Reference

** Diff(Cri) = (Power by Critical spectrum - Reference)/Reference

Figure 10. The assembly-wise power distribution for PWR 3D core problem

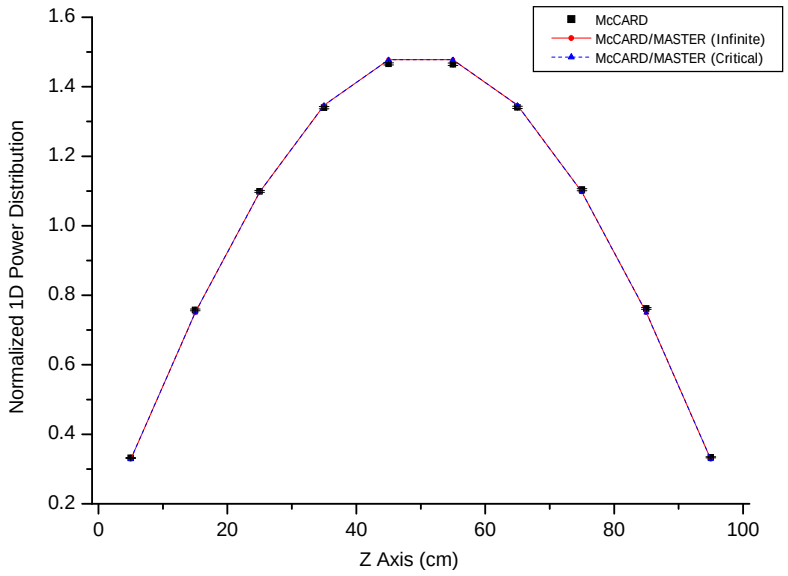

Figure 11. The average axial power distribution for PWR 3D core problem

3. CONCLUSIONS

It is simple and straightforward to generate few group reaction cross sections by MC codes. Yet generation of few group diffusion coefficients is not so simple and has been a tricky issue in generating few group constants by MC codes. Some studies have suggested computing group-wise diffusion coefficients in the same way as group-wise reaction cross sections simply by tallying the transport rate, i.e., the integral of transport cross sections derivable from P_1 theory multiplied by neutron flux over the corresponding energy range and over the spatial volume to be homogenized [8, 9]. Because these studies have not discussed about qualifications of such few group constants in terms of the core neutronics calculations, there is no knowing how good they are. To our earlier experience with such few group constants for PWR FAs, however, the reaction rate cross sections are similar to those from deterministic FA codes like HELLIOS and CASMO but diffusion coefficients are far off those from deterministic codes. Contrary to this experience, it has been shown already that the few group constants from the MC method are similar to those from HELLIOS code [5]. In addition to this, excellent agreements between MC analysis by McCARD and two-step McCARD/MASTER analysis for both a mini-PWR and a realistic PWR core neutronics shown in this paper are a clear manifestation of the qualification of the MC method as a reliable few group constant generator.

The MC method as a few group constant generator has a few inherently superior features, compared with its deterministic counterpart. The former does not require the multi-group approximation while the latter does as used in all of the deterministic production codes today. The former does not involve any complication in preparing continuous energy data from the evaluated nuclear data inputs, while the latter requires a sophisticated preprocessing of in-built multi-group cross section data to prepare proper self-shielded cross sections matching each

material composition – preferably with the guidance of experimental data on the neutronics behavior of the fuel and/or core systems – and thus to ensure the desired accuracy of ensuing core neutronics calculations. The former can model the geometry and the material arrangement of a given nuclear system exactly in the way it is designed, while the latter sometimes finds it difficult to do so in such nuclear systems like high temperature gas-cooled reactor systems which adopts fuel particles. Because of these features, the former is expected to bring about more accurate two-step core neutronics analysis than the latter. Also, the former is preferred to the latter in the neutronics analysis of brand new nuclear systems like some of GEN IV reactors experimental data on neutronics behavior of which are unavailable.

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REFERENCES

1. Y. Kim and W. S. Park, “Reactivity-Equivalent Physical Transformation for Elimination of Double Heterogeneity,” *Trans. Am. Nucl. Soc.*,**93**, p.959 (2005).
2. Allen F. Henry, “Nuclear-Reactor Analysis,” The MIT Press, Cambridge (1975).
3. H. J. Shim et al.,“Generation of Few Group Diffusion Theory Constants by Monte Carlo Code,” *Trans. Am. Nucl. Soc.*, **99**, p.343 (2008).
4. R. J. J. Stamm’ler et al., “Helios Methods,” Scandpower (1994).
5. H. J. Park et al., “Assembly Depletion with Critical Spectrum in McCARD Monte Carlo Calculations and Comparison with HELIOS,” *PHYSOR 2010*, Pittsburgh, USA, May 9-14 (2010).
6. B. O. Cho et al., “MASTER-2.0: Multi-purpose Anlayzer for Static and Transient Effect of Reactor,” KAERI/TR-1211/99 (1997).
7. R. J. J. Stamm’ler and M. J. Abbate, “Methods of Steady-State Reactor Physics in Nuclear Design,” Academic Press, London (1983).
8. G. Ilas and F. Rahnema, “A Monte Carlo based nodal Diffusion Model for Criticality Analysis of Spent Fuel Storage Lattice,” *Ann. Nucl. Eng.*,**30**, pp.1089 (2003).
9. M. Tohjoh et al.”Application of continuous-energy Monte Carlo code as a cross section generator of BWR core calculations,” *Ann. Nucl. Eng.*, **32**, pp.857-875 (2005).