# Monte Carlo Few Group Constants Generation Considering the Free-Monatomic-Gas Models

Ho Jin Park a\* and Hyung Jin Shimb

<sup>a</sup>Korea Atomic Energy Research Institute, 989-111 Daedeok-Daero, Yuseong-gu, Daejeon, Korea <sup>b</sup>Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 151-742, Korea <sup>\*</sup>Corresponding author: parkhj@kaeri.re.kr

# 1. Introduction

Recently, in order to handle complex geometric information data and treat the continuous energy nuclear data directly, the few group diffusion theory constants are generated by the Monte Carlo (MC) code such as McCARD[1,2]. To generate a group-to-group scattering cross section on MC particle simulation, a thermal motion between a neutron and a target atom would be considered. McCARD provides two other schemes - application of thermal scattering cross section libraries and the free-monatomic-gas models. To consider the effect of Doppler broadening by cell temperatures, the Doppler-broadening rejection correction (DBRC) method[3] is implemented into McCARD.

In this study, the few group constants are generated by McCARD code with the MC free gas thermal treatment models and qualified by comparing reference with two-step calculations.

## 2. Methods and Results

#### 2.1 MC Free Gas Thermal Treatment

The group-to-group scattering cross section defined by

$$\Sigma_{gg'} = \frac{\int_{V} \int_{\Delta E_{g'}} \int_{AE_{g'}} \int_{4\pi} \Sigma_{s}(\mathbf{r}, E' \to E) \phi \ (\mathbf{r}, E', \Omega) d\Omega dE' dE d\mathbf{r}}{\int_{V} \int_{\Delta E_{g'}} \int_{4\pi} \phi \ (\mathbf{r}, E, \Omega) dE d\mathbf{r}}$$
(1)

$$\Sigma_{s}(\mathbf{r}, E' \to E) = \Sigma_{s}(\mathbf{r}, E', \Omega', T(\mathbf{r})) f_{s}(E' \to E, \Omega' \to \Omega, T(\mathbf{r}))$$
<sup>(2)</sup>

where  $\Sigma_s(\mathbf{r}, E' \to E)$  and  $\phi(\mathbf{r}, E', \Omega)$  are the double differential scattering cross section and the angular flux, respectively. Though all the neutron cross sections should be Doppler-broadened by the cell temperatures,  $f_s(E' \to E, \Omega' \to \Omega, T(\mathbf{r}))$  taken from NJOY[4] code are independent of temperature. In order to correct this problem, the free-monatomic-gas models are implemented by sampling the target nucleus's velocity vector and using the relative neutron energy in the MC simulation of the collision kernel. The default model for the Doppler-broadening of scattering kernel in McCARD is the constant cross section method which is applied when the neutron energy is lower than 400kT or the sampled target nucleus is hydrogen. For the exact model, the rejection process for the probability of scattering reaction for the relative velocity between neutron and target atom should be accompanied with the sampling algorithm of the constant cross section model by the DBRC method and the weight correction model[5]. Figure 1 shows the algorithm of MC simulation considering the free-monatomic-gas models.



Fig. 1. Algorithm of MC simulation with free gas thermal treatment

2.2 Qualification of Few-Group Constants by MC method

To investigate the qualification of the group-to-group scattering cross section generated by McCARD, the depletion analyses for the two PMR-200[6] fuel block problems are conducted. One is the fuel block with the burnable poison (BP) hole filled with graphite and the other is that with B<sub>4</sub>C BP. The 10-group few-group cross sections are used to calculate the  $k_{inf}$  of the PMR-200 fuel blocks by McCARD/MASTER over burnup. All the McCARD calculations are performed with 200 active and 20 inactive cycles with 10,000 neutron particles per a cycle. Figure 2 and 3 show the McCARD/MASTER results in comparison with reference McCARD calculations. The two calculations for  $k_{inf}$  are in excellent agreements. The RMS difference

of the fuel block without  $B_4C$  BP between two calculations is 74 pcm while that with  $B_4C$  BP is 73 pcm.



Fig. 2. *k<sub>inf</sub>* versus burnup for PMR-200 fuel block w/o BP rods



Fig. 3. kinf versus burnup for PMR-200 fuel block w/ BP rods

# 2.3 Effect of the DBRC Method

Table I shows the FTCs of PWR fuel assembly (FA) calculated by the two-step McCARD/MASTER for each sampling model. It can be observed from these results that the DBRC model makes FTC more negative by about 15%. Table II provides the two-group constants in 1100K. The fast-group absorption cross section ( $\Sigma_{a1}$ ) shows significant differences and is observed as the most significant contributor to  $\Delta k_{inf}$  between two models.

Table I: Comparison of FTCs for PWR FA in DBRC model

Temp	Constants XS Model		DBRC Model	
(Kelvin)	$\mathbf{k}_{\mathrm{eff}}$	FTC (pcm/K)	k <sub>eff</sub>	FTC (pcm/K)
700	1.33557	2.02	1.33454	2.26
1100	1.32390	-2.92	1.32112	-3.30
2000	1.30192	-2.44	1.29538	-2.86

Table II: Two-group constants for PWR FA (1100K)

Case	Constants XS Model	DBRC Model	$\Delta k_{inf} (\Delta \Sigma)^*$
$\Sigma_{a1}$	9.451×10 <sup>-3</sup>	9.489×10 <sup>-3</sup>	197
$\Sigma_{a2}$	$7.957 \times 10^{-2}$	7.956×10 <sup>-2</sup>	-16
$v\Sigma_{f1}$	6.765×10 <sup>-3</sup>	6.755×10 <sup>-3</sup>	38
$v\Sigma_{f2}$	1.341×10 <sup>-1</sup>	1.341×10 <sup>-1</sup>	19
$\Sigma_{s12}$	$1.594 \times 10^{-2}$	1.591×10 <sup>-2</sup>	38
$\Sigma_{s21}$	$2.599 \times 10^{-4}$	$2.605 \times 10^{-4}$	0
k <sub>inf</sub> (MC)	1.32413± 0.00019	1.32095± 0.00018	0.00318
$k_{inf}(2grp)$	1.32390	1.32112	0.00278

 $_{inf} (\Delta \Sigma) = k_{inf} (\Sigma)$ 

# 3. Conclusions

The two-step analysis using few group constants by MC method considering the MC free gas treatments including DBRC model are performed in this paper. The results of two-step McCARD/MASTER analysis for the PMR-200 which has a highly complex structure are clear manifestations of the qualification of the few group constants calculated by MC method. And the few group constants with the exact scattering model such as the DBRC model employed in the McCARD code are easily generated without additional processing.

By showing excellent agreement between McCARD and McCARD/MASTER, it is confirmed that the MC method as the few-group constants generator has superior features compared the deterministic method which require a sophisticated preprocessing of in-built multi-group cross section with DBRC method.

#### REFERENCES

[1] H. J. Park, H. J. Shim, and C. H. Kim ,"Generation of Few-Group Diffusion Theory Constants by Monte Carlo Code McCARD," Nuclear Science and Engineering **172**, p66-77 (2012)

[2] H. J. Shim, B. S. Han, J. S. Jung, H. J. Park, and C. H. Kim, "McCARD: Monte Carlo Code for Advanced Reactor Design and Analysis," Nuclear Engineering and Technology **44**, p161, (2012)

[3] B. Becker, "On the influence of the Resonances Scattering Treatment in Monte Carlo Codes on High Temperature Reactor Characteristics," Ph.D. Thesis, University Stuttgart, Jun. 2010 (2010)

[4] R. E. MacFarlance, D. W. Muir, R. M. Boicourt, "The NJOY Nuclear Data Processing System, Volume I:User Manual," LA-9303-M, ENDF-324, Los Alamos National Laboratory (1982)

[5] D. J. Lee, K. Smith, J. Rhodes, "The impact of 238U Resonance Elastic Scattering Approximations on Thermal Reactor Doppler Reactivity," Annals of Nuclear Energy **36**, p274-280. (2009)

[6] H. C. Lee et al, "Decay Heat Analysis of VHTR Cores by Monte Carlo Code Depletion Calculation," Annals of Nuclear Engineering **37**, p1356 (2010)