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Application of Higher Order Fission Matrix for Real Variance Analysis in McCARD Monte Carlo Eigenvalue Calculation

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Abstract - *In order to predict the real to apparent standard deviation (SD) ratio for a local tally, the Endo's theoretical model based on auto-regressive (AR) model was applied to a non-analog Monte Carlo (MC) eigenvalue calculation. The eigenvectors and eigenvalues of a higher mode fission matrix (HOFM) for the theoretical model were calculated by using the Hotelling deflation method. In this study, the HOFM capability was implemented into McCARD, which is non-analog MC code. In case that the number of cycles is small, there is no significant difference between reference calculation and the theoretical model. As the number of cycles increases, a considerable difference between the two appeared. Furthermore, to examine the difference between analog and non-analog MC results, real to apparent SD ratios are calculated by using an in-house MC code Roulette and MCNP. It is noted that a difference in the MC and theoretical results with large cycle number still exists for both of two. In the near future, the research to explain the discrepancy between the theoretical model and the reference results by the non-analog MC calculation will be carried out.*

I. INTRODUCTION

In a Monte Carlo (MC) eigenvalue calculation, it is well known that the apparent variance of a local tally such as a pin power differs from the real variance considerably whereas the difference in a global tally such as k-effective is negligible. In the previous studies [1,2], the difference of the real to apparent standard deviation (SD) ratio was investigated for the tally size in the MC eigenvalue calculations with a realistic problem such as the BEAVRS [3] benchmark. It was noted that the apparent variance of a local MC tally such as pin-wise fission power or fuel assembly (FA)-wise fission power tends to be smaller than the real value while an apparent variance of the global MC tally such as k_{eff} is similar to the reference value. In slowly convergent problems with high dominance ratio (DR), the real to apparent SD ratio for a local tally would be more than one hundred.[1] Therefore, the prediction for a real to apparent SD ratio is very important in terms of a whole core MC analysis. Meanwhile, the MC method in eigenvalue calculations uses a power iteration method. In the power iteration method, the fission matrix (FM) and fission source density (FS) are used as the operator and solution. The FM is useful to estimate a variance and the covariance because the FM can be calculated by a few cycle calculations even at the inactive cycle. Recently, T. Endo et al. proposed a theoretical model to predict the underestimation ratio for a local tally [4,5]. It was derived on the basis of a higher order fission matrix (HOFM) and the autoregressive (AR) model in the MC eigenvalue calculations. In the infinite slab problem, the apparent to real SD ratios of fission rate tallies calculated by the formulation agree well with those by the analog MC calculation. The purpose of this work is to implement the HOFM capabilities into McCARD [6] and to investigate the real to apparent SD ratios for non-analog MC calculation with the aid of the HOFM and the theoretical model. In the MC eigenvalue calculation, the HOFM can be easily calculated from the FM by using the hotelling deflation method [7,8].

II. HIGHER ORDER FISSION MATRIX

1. Higher Order Fission Matrix in MC Eigenvalue Calculation

A standard form of the Boltzmann transport equation can be rewritten as

$$S = \lambda \mathbf{H} S, \tag{1}$$

where S and $\mathbf{H}$ are the FS and fission operator, respectively. S is defined by $S \equiv \mathbf{F}\phi$ while $\mathbf{H}$ is defined by $\mathbf{H} \equiv \mathbf{F}\mathbf{T}^{-1}$. $\mathbf{T}$ and $\mathbf{F}$ denote the net loss and fission production operator in the standard form of the Boltzmann transport equation. The other notations are ordinary one. S can be expressed as follows:

$$\begin{aligned} S^{(c)}(\vec{r}) &= \int_0^\infty \nu\Sigma_f(\vec{r},E)\phi^{(c)}(\vec{r},E)dE \\ &= \sum_{n=0}^{N} a_n^{(c)} S_n(\vec{r}), \\ S_n(\vec{r}) &\equiv \int_0^\infty \nu\Sigma_f(\vec{r},E)\phi_n(\vec{r},E)dE, \end{aligned} \tag{2}$$

where $S^{(c)}(\vec{r})$ is the FS at the c-th cycle and $\phi^{(c)}(\vec{r},E)$ is the flux at the c-th cycle. $\phi_n(\vec{r},E)$ and $S_n(\vec{r})$ is the flux and the FS of the *n*-th mode, respectively. $a_n^{(c)}$ is the expansion coefficient of the *n*-th mode with the FS at the *c*-th cycle. Using the orthogonality of the eigenvectors, the expansion coefficient can be calculated by

$$a_n^{(c)} = \frac{\langle S(\vec{r}) S_n^T(\vec{r}) \rangle}{\langle S_n(\vec{r}) S_n^T(\vec{r}) \rangle}. \quad (3)$$

In the MC method, the $S_n(\vec{r})$ can be calculated by the hotelling deflation method. The deflated fission matrix for the *n*-th mode is

$$\mathbf{H}_n = \mathbf{H} - \sum_{n'=0}^{n-1} \frac{1}{\lambda_{n'}} \cdot \frac{S_{n'} S_{n'}^T}{\langle S_{n'} S_{n'}^T \rangle}. \quad (4)$$

A module for the HOFM calculations was implemented into McCARD.

2. Verification of Higher Order Fission Matrix Calculation Module

Table I. *k*-eigenvalues calculated by McCARD

Mode	MATLAB	McCARD	
		k_n	$\sigma(k_n)/k_n$ (%)
0	0.999438	0.999438	0.003
1	0.997250	0.997250	0.004
2	0.993416	0.993416	0.004
3	0.987999	0.987999	0.004
4	0.981009	0.981009	0.004
5	0.972567	0.972567	0.004
6	0.962663	0.962663	0.004
7	0.951415	0.951415	0.004

To examine the newly implemented HOFM routines, a one-group slab homogeneous problem surrounded by a thin reflector was used. This slab problem was taken from reference 9. The length of the central fissile region is 200 cm while the length of the left and right reflector region is only 5 cm. The central fissile regions were divided equally into 50 mesh regions for the tally. The MC eigenvalue calculations were performed on 2,500 total cycles with 1,000,000 neutron histories per cycle and 1,500 inactive cycles. Table I compares the k-eigenvalues calculated by the McCARD and MATLAB scripts. The SD of the *n*-th mode k-eigenvalue, k_n, was estimated from 25 replicas with different random number sequence. The agreement between the McCARD and MATLAB seems excellent for each mode. From the results, the dominance ratio (k_1/k_0) can be found to be about 0.998. Figure 1 shows the eigenfunctions calculated by McCARD. The results by MATLAB was omitted in Fig 1 because they showed an excellent agreement with those by McCARD for each mode, they are omitted in Fig 1.

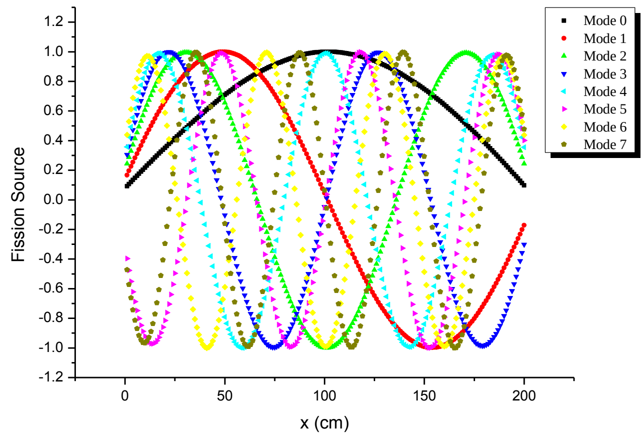

Fig. 1. Higher-order mode eigenfunctions of 1D slab problem

III. REAL TO APPARENT SD RATIO ESTIMATION BY AR MODEL

1. Derivation of the Real to Apparent SD Ratio by AR Model

In this section, the real to apparent SD ratio for a local fission rate tally will be derived by using the same way that Endo et al formulated [4]. The Endo's notations were referred to in the following derivations. The cycle-wise expansion coefficients of FS, $a_n^{(c)}$, by the AR model can be expressed as

$$\begin{aligned} a_n^{(c)} &\approx \frac{k_n}{k_0} a_n^{(c-1)} + d_n^{(c)} \\ &\equiv \rho_n a_n^{(c-1)} + d_n^{(c)}, \end{aligned} \quad (5)$$

where $d_n^{(c)}$ indicates the expansion coefficients of *n*-th mode in the noise term for *c*-th cycle and ρ_n is defined by k_n/k_0. The k_n's are ordered such that $k_0 > |k_1| > |k_2| > \cdots$. The variance and auto-covariance of the expansion coefficients can be calculated by

$$\sigma^2\left[a_n^{(i)}\right] \approx \frac{\sigma_{d_n}^2}{1-\rho_n^2} \equiv \sigma_{a_n}^2, \quad (6)$$

$$\begin{aligned}&\mathrm{cov}[a_n^{(i)}, a_n^{(i+j)}]\\ &= E\left[a_n^{(i)}a_n^{(i+j)}\right] - E\left[a_n^{(i)}\right]E\left[a_n^{(i+j)}\right] \\ &= \rho_n^j \frac{\sigma_{d_n}^2}{1-\rho_n^2} = \rho_n^j \sigma_{a_n}^2,\end{aligned} \tag{7}$$

where i and j are cycle indices and $\sigma_{d_n}^2$ is the variance of $d_n^{(c)}$. The real or true variance of the expansion coefficients of the n-th mode can be calculated by using Eq.(6) and (7).

$$\begin{aligned}\sigma_R^2\left[\bar{a}_n\right] &= \frac{1}{N}\sigma^2\left[a_n^{(i)}\right] + \frac{1}{N^2}\sum_i^N \sum_{\substack{j \\ i\neq j}}^N \mathrm{cov}[a_n^{(i)}, a_n^{(j)}] \\ &= \frac{1}{N}\left(\sigma_{a_n}^2 + \frac{2}{N}\sum_j^{N-1}(N-j)\mathrm{cov}[a_n^{(i)}, a_n^{(j)}]\right) \\ &= \frac{\sigma_{a_n}^2}{N}\left(1 + \frac{2\rho_n(\rho_n^N + N(1-\rho_n)-1)}{N(1-\rho_n)^2}\right),\end{aligned} \tag{8}$$

where N is the number of cycles. The apparent variance of $\bar{a}_n$, $\sigma_A^2\left[\bar{a}_n\right]$, which is defined as the expected value of the sample variance, can be calculated by

$$\begin{aligned}\sigma_A^2\left[\bar{a}_n\right] &= \frac{1}{N}\sigma^2\left[a_n^{(i)}\right] - \frac{1}{(N-1)N^2}\sum_i^N \sum_{\substack{j \\ i\neq j}}^N \mathrm{cov}[a_n^{(i)}, a_n^{(j)}] \\ &= \frac{1}{N}\left(\sigma_{a_n}^2 - \frac{2}{N(N-1)}\sum_j^{N-1}(N-j)\mathrm{cov}[a_n^{(i)}, a_n^{(j)}]\right) \\ &= \frac{\sigma_{a_n}^2}{N}\left(1 - \frac{2\rho_n(\rho_n^N + N(1-\rho_n)-1)}{N(N-1)(1-\rho_n)^2}\right).\end{aligned} \tag{9}$$

Meanwhile, the fission source rate at a tally region V_m can be expressed by using Eq.(2).

$$\begin{aligned}S^m &= \int_{V_m}\int_0^\infty \nu\Sigma_f(\vec{r},E)\phi(\vec{r},E)dEdV = \sum_{n=0}^N w_n a_n, \\ &\textit{where } w_n \equiv \int_{V_m}\int_0^\infty \nu\Sigma_f(\vec{r},E)\phi_n(\vec{r},E)dEdV.\end{aligned} \tag{10}$$

From Eq.(10), the real to apparent SD ratio of fission rate tally can be written as

$$\frac{\sigma_R\left[\overline{S^m}\right]}{\sigma_A\left[\overline{S^m}\right]} \approx \sqrt{\frac{\sum_{n=1}^O \frac{w_n^2}{1-\rho_n^2}\left(1 + \frac{2\rho_n(\rho_n^N + N(1-\rho_n)-1)}{N(1-\rho_n)^2}\right)}{\sum_{n=1}^O \frac{w_n^2}{1-\rho_n^2}\left(1 - \frac{2\rho_n(\rho_n^N + N(1-\rho_n)-1)}{N(N-1)(1-\rho_n)^2}\right)}}. \tag{11}$$

where O is the upper limit number of modes. In the case that number of total cycle, N, approaches infinity, the real to apparent SD ratio can be finally rearranged by

$$\frac{\sigma_R\left[\overline{S^m}\right]}{\sigma_A\left[\overline{S^m}\right]} \approx \sqrt{\frac{\sum_{n=1}^O \left(\frac{w_n^2}{1-\rho_n^2}\right)\cdot\left(\frac{1+\rho_n}{1-\rho_n}\right)}{\sum_{n=1}^O \left(\frac{w_n^2}{1-\rho_n^2}\right)}}. \tag{12}$$

2. Application of Theoretical Model with Non-Analog MC HOFM Solution

In order to examine the formulation derived in the previous section, the benchmark tests for simple slab problems were performed using the HOFM capability implemented into McCARD. The simple slab problems were taken from reference 4.

Table II: Cross Section in the slab problem [4]

Problem	B.C.* for both side	Σ_t	$\Sigma_{s,0}$	$\nu\Sigma_f$
I	Reflective	1.0	0.6	0.48
II	Vacuum	1.0	0.6	0.48

* B.C. = Boundary Condition

Table II shows a detailed description for the slab problems. The width of the slab is 10 cm. In problem I, the analytic solution for ρ_n and $S_n(\vec{r})$ is as below:

$$\rho_n \equiv \frac{k_n}{k_0} = \frac{\Sigma_a}{\left(1/3\Sigma_t\right)\left(n\pi/10\right)^2 + \Sigma_a}, \tag{15}$$

$$S_n(x) = \begin{cases}\cos\left(\frac{n\pi}{10}x\right), & (\text{n=0,2,4,}\cdots) \\ \sin\left(\frac{n\pi}{10}x\right), & (\text{n=1,3,5,}\cdots)\end{cases}, \tag{16}$$

where Σ_t and Σ_a are the macroscopic total cross section and absorption cross section, respectively. Figure 2 shows the real to apparent SD ratios of the cell-wise fission rate tally by the theoretical models with the analytic solutions, and with the non-analog MC HOFM solutions for problem I. In that case, the number of meshes is set as 10. The reference solutions were calculated by using the 200,000 neutron histories per cycle and 5 active cycles. The number of inactive cycles is 1,000. To obtain the reference solutions for the real to apparent SD ratio, the 1,000 McCARD eigenvalue calculations were performed using different random number seeds. In Fig 2, N and O are the number of the cycles and the upper limit number of the mode contributed for the real to apparent SD ratio prediction, respectively. The real to apparent SD ratio by theoretical model was calculated using Eq.(12). At the central region, there is no significant difference between reference and theoretical model. However, we can observe that the real to apparent SD ratios at boundary region are not in good agreement.

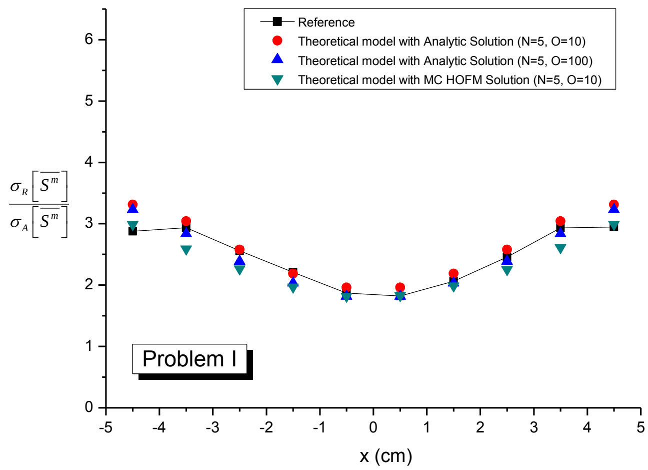

Fig. 2. Real to Apparent SD ratio of Fission Rate Tallies (Problem I)

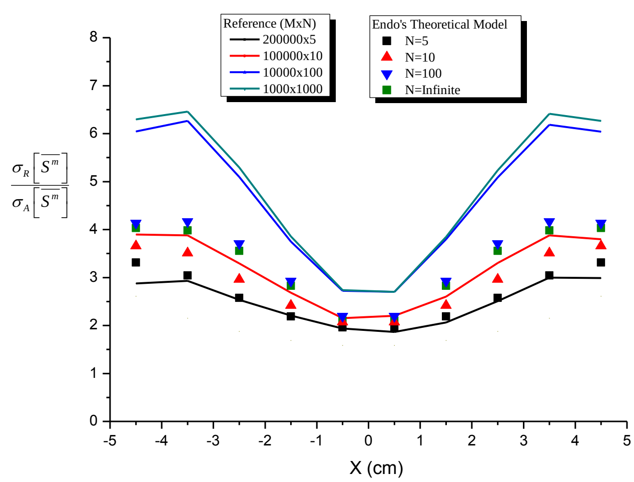

Fig. 3. Real to Apparent SD ratio of Fission Rate Tallies due to neutron history condition in MC calculations (Problem I)

Figure 3 shows the results by the theoretical models and the reference solutions with the various neutron history conditions. *M* and *N* indicate the number of neutron histories per cycle and the number of active cycles. The number of total histories was fixed as 1,000,000. The detailed calculation condition for the reference calculations are shown as follow:

- Total number of neutron histories : 1,000,000 (fixed)
- Number of inactive cycles : 1,000
- Case (number of active cycles) : 5, 10, 100, 1,000
- Non-analog MC calculations with implicit capture

In Fig. 3, the solid lines indicate the reference MC solution while the dots present the results of the theoretical model calculated by using Eq.(11) and Eq.(12). As the *N* approaches infinity (∞), the real to apparent SD ratio of the theoretical model at the outermost region is converged to 4.0 whereas the reference is converged to 6.5. This figure shows that the Eq.(12) with large *N* is no longer applicable. Figure 4 shows the real to apparent SD ratios of fission rate tally by the theoretical models with the non-analog MC HOFM solutions for problem II. The conditions for the reference and the HOFM calculations are exactly same. Overall, the results of problem II are similar to those of problem I.

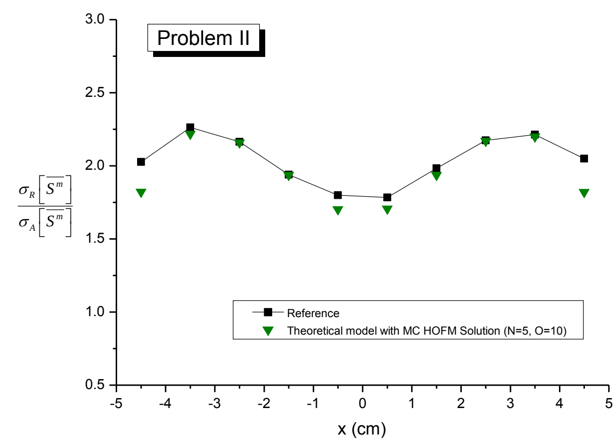

Fig. 4. Real to Apparent SD ratio of Fission Rate Tallies (Problem II)

3. Comparison between Analog and Non-Analog MC HOFM Solution

To examine the difference between analog and non-analog MC results, an in-house multi-group MC code – Roulette is developed. Roulette can be used for both analog and non-analog mode calculations. In the non-analog mode, the implicit capture method, which is also known as survival biasing, was used with Russian roulette technique. In this mode, a neutron is absorbed by weight reduction and a fission source is sampled at each collision site. In the analog mode, a neutron is killed by absorption and a fission source is sampled after the fission event is explicitly determined [10,11]. MCNP [12] can handle both analog and implicit absorption for neutron particles. For comparison with

Roulette, MCNP calculations are additionally performed. The detailed calculation conditions are shown as follow:

- Total number of neutron histories : 1,000,000 (fixed)
- Number of inactive cycles : 100
- Number of active cycles (N) : 10, 1000
- Number of MC calculations for case : 100
- MC Calculation Case :
  1) McCARD (implicit capture)
  2) Roulette (implicit/analog mode)
  3) MCNP (implicit/analog absorption)

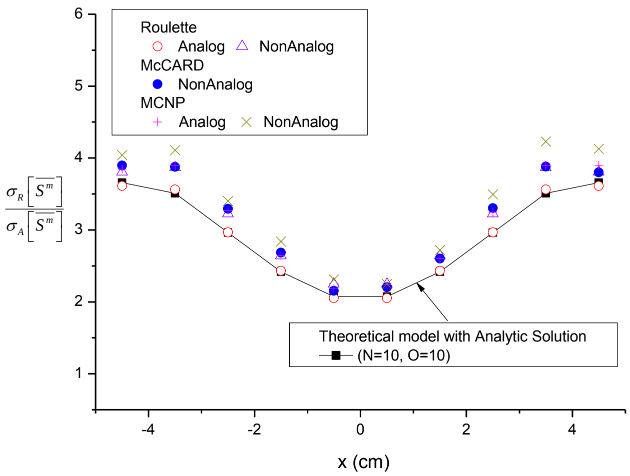

Fig. 5. Comparison of Real to Apparent SD ratio between Analog and Non-Analog Results at N=10 (Problem I)

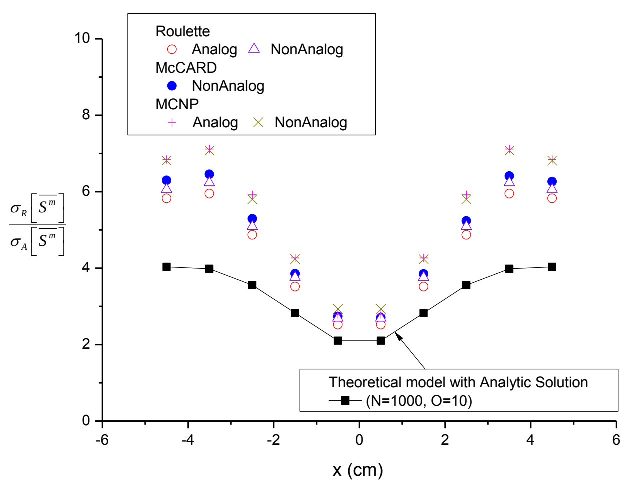

Fig. 6. Comparison of Real to Apparent SD ratio between Analog and Non-Analog Results at N=1000 (Problem I)

Figure 5 and 6 compare the difference between the analog and non-analog MC results for the real to apparent SD ratio of fission rate tallies in problem I, which is described in Table II. The results by the theoretical model are calculated by Eq. (11) using the analytic solution (O=10). In either N case, there are no meaningful discrepancy between analog and non-analog results. As shown in Fig 6, it is noted that a difference in the MC and theoretical results with large N still exists for all calculation cases.

IV. PRELIMINARY STUDY FOR PRACTICAL PROBLEM

In this section, the prediction accuracy of the theoretical model with MC HOFM solutions for real to apparent SD ratio is examined by means of a 2D core problem with 57 FAs for SMR (Small Modular Reactor) [13]. Figure 7 shows the fuel loading pattern for the 2D octant SMR core. It has six types of 17x17 FAs: L1, L2, H1, H2, H3, and H4, which differ from one another in the U^{235} enrichment and the number of Gd_2O_3-UO_2 fuel rods. Figure 8 presents the configuration of FA for each type.

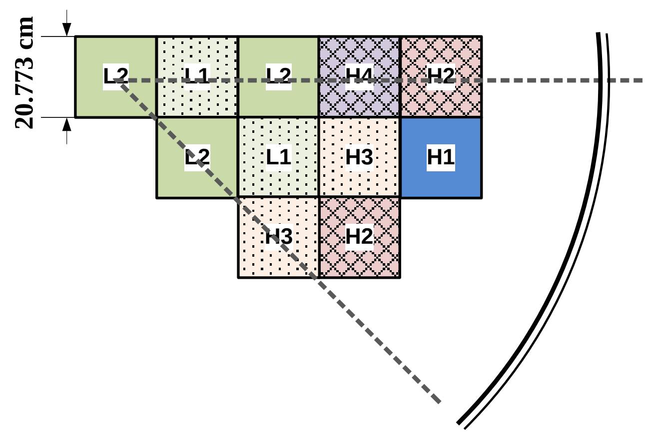

Fig. 7. Fuel loading pattern for 2D SMR core

For the theoretical model calculations, the MC HOFM solutions are calculated by McCARD. To form the FM for octant SMR core, FA-wise regional discretization was introduced. For this reason, as shown in Fig 7, the dimensions of its FM is determined as 11x11. And its dominance ratio (k_1/k_0) is about 0.841. To obtain its reference solutions, one hundred McCARD calculations were performed using different random number sequence. The neutron history condition is as below:

- Total number of neutron histories : 1,000,000 (fixed)
- Number of inactive cycles : 100
- Number of active cycles (N) : 5

Figure 9 and 10 compare the real to apparent SD ratio of FA-wise fission power tally for the theoretical model and reference in each N case, respectively. At L1(1,1) and L1(2,3) FA, the theoretical model produce the real to apparent SD ratios with relative errors larger than 30%.

Nonetheless, there are interesting points to observe. It seems that the overall shape of the real to apparent SD ratios by the theoretical model appear to follow the one of the reference.

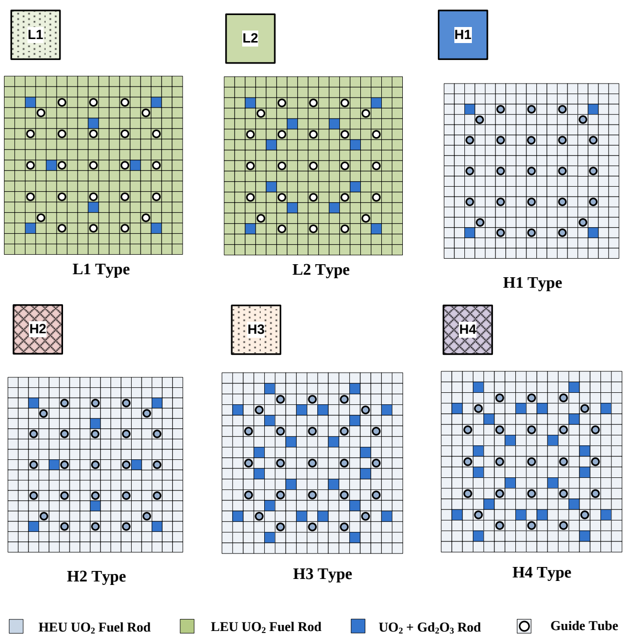

Fig. 8. Configuration of fuel assemblies in 2D SMR core

L2(1,1)	L1(1,2)	L2(1,3)	H4(1,4)	H2(1,5)	Name [a)]
2.166	2.449	1.717	1.614	2.261	Ref [b)]
1.335	2.402	1.746	1.583	1.984	Theo.[c)]
-0.38	-0.02	0.02	-0.02	-0.12	Diff. [d)]
	L2(2,2)	L1(2,3)	H3(2,4)	H1(2,5)	
	1.942	1.619	1.726	2.187	
	2.130	2.220	1.944	2.810	
	0.10	0.37	0.13	0.28	
		H3(3,3)	H2(3,4)		
		1.678	1.987		
		1.608	2.313		
		-0.04	0.16		

a) Name of FA consists of its type and location.
b) Reference Real to Apparent SD Ratio by McCARD.
c) Theoretical Real to Apparent SD Ratio with MC HOFM solution.
d) Diff. = (Theo.-Ref.)/Ref.

Fig. 9 Real to Apparent SD ratio of FA-wise power for a 2D octant SMR core (N=5)

V. CONCLUSIONS

In this study, the HOFM capability using the hotelling deflation method was implemented into McCARD and used to predict the behavior of a real to apparent SD ratio. In order to predict the real to apparent SD ratio, the application of the theoretical model based on the AR model was conducted. In the Endo's study, the theoretical model predicted well the reference solution calculated by analog MC code. In the study, the two slab benchmarks and 2D octant SMR core are performed for validation and verification using Roulette, MCNP, and McCARD code. Whether the MC code uses analog or non-analog algorithm, in case that the number of cycles is small, there is no significant difference between reference calculation and the theoretical model. However, as the number of cycles increases, a considerable difference between the two appeared. In the large cycle number case, it is assumed that the seemingly difference value stem from the inter-cycle correlation [14] or the approximation of the derived formulation for the theoretical model, such as not considering the correlation of the expansion coefficients among different modes. In the near future, the research to explain the discrepancy between the theoretical model and the reference results with the large cycle number will be carried out. Furthermore, the practical application for a high dominance ratio problem such as the BEAVRS benchmark will be conducted.

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