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VERA Pin and Fuel Assembly Depletion Benchmark Calculations by McCARD and DeCART

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1. Introduction

Monte Carlo (MC) codes have been developed and used to simulate a neutron transport since MC method was devised in the Manhattan project. Solving the neutron transport problem with the MC method is simple and straightforward to understand. Because there are few essential approximations for the 6-dimension phase of a neutron such as the location, energy, and direction in MC calculations, highly accurate solutions can be obtained through such calculations. However, massive computational resources are needed to obtain a precise solution. In the early days, the costs and capabilities of the hardware and software had a limited use of the MC method in a nuclear design analysis. Based on the recent development of computational performance, the application of the MC method is extended to a whole core and depletion analysis.

In a previous study [1], new procedures were introduced to improve the DeCART [2] multi-group cross section library generation system, and new DeCART libraries were generated using ENDF/B-VII.1 evaluated nuclear data library. The results for a small modular reactor (SMR) analysis show that the DeCART calculations with new generated libraries give quite good agreements with the reference McCARD [3] solutions.

Meanwhile, various benchmarks for a verification of the prediction capabilities in a depletion analysis have been developed and executed. Recently, The VERA depletion benchmark problems [4] based on the "The VERA Core Physics Benchmark Progression Problem" have been introduced from Oak Ridge National Laboratory (ORNL), which provided detailed guidelines including the burnup chain data for a depletion analysis. As a part of an I-NERI Project, Seoul National University (SNU), Ulsan National Institute of Science and Technology (UNIST), and ORNL have performed these benchmark calculations using their neutronic transport codes.

In this work, the VERA pin and fuel assembly (FA) depletion benchmark calculations are performed to examine the depletion capability of the newly generated DeCART multi-group cross section library. To obtain the reference solutions, MC depletion calculations are conducted using McCARD. Moreover, to scrutinize the effect by stochastic uncertainty propagation, uncertainty propagation analyses are performed using a sensitivity and uncertainty (S/U) analysis method and stochastic sampling (S.S) method.

2. VERA Depletion Benchmark Analysis

2.1 VERA Depletion Benchmark

In this study, pin and FA depletion benchmark problems were selected from the benchmarks [4]: 1C and 2C. A pin pitch of 1.26 cm, cladding outer radius of 0.4750 cm, and pellet radius of 0.4096 cm are common to all VERA benchmarks. The FA consists of a 17x17 lattice array of 264 UO_2 fuel pins and 25 empty guide tubes and its pitch is 21.5 cm. The power density is 40.0 W/gU. The temperature in the fuel region is 900K while that in the other regions is 600K. The fuel pellet region is divided into three sub-regions to consider its radial power distributions for burnup analyses.

Figure 1 shows the configuration of fuel pin and FA problem. The detailed specifications of each problem are briefly described in reference 4.

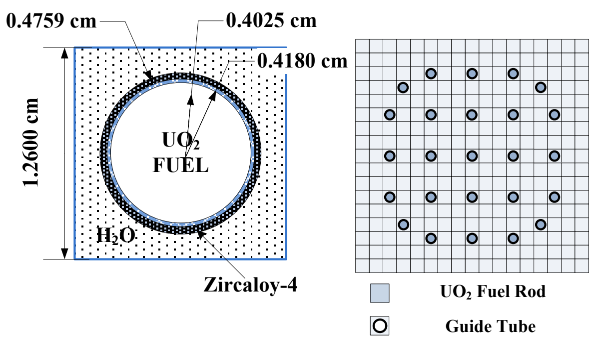

Fig. 1. Configuration of Pin Cell and FA Problem

2.2 Numerical Results for VERA Depletion Benchmark

The VERA depletion benchmark calculations were performed using the McCARD and DeCART codes. In all DeCART calculations, the direct iteration method with a resonance integral table (DRI) [5] for the resonance treatment and PV01-47G library generated by the improved procedure [1] were used in common. In the improved procedure, the resonance interference between U^{235} and U^{238} were only considered in the stage of the resonance integral (RI) generation. To consider the resonance interference among other actinides and fission products (FP), the resonance interference procedure in the DeCART code was used as before. To obtain the MC reference solution, McCARD depletion analyses were performed with 10,000 neutron histories per cycle, 50 inactive cycles, and 500 active cycles for each depletion time step (DTS). For all of the calculations, thermal hydraulic feedback was not considered and P_2 transport approximation was applied. Figures 2 and 3 show the infinite multiplication factors (k_{inf}) calculated by McCARD and DeCART for the pin (1C) and FA (2C) problems, respectively. In these calculations, a conventional semi predictor-corrector (P-C) method was only used. Based on the McCARD reference solutions, the DeCART calculation for the pin problem gives an RMS (Root Mean Square) difference of 61 pcm over the burnup, whereas the RMS difference for the FA problem is 47 pcm.

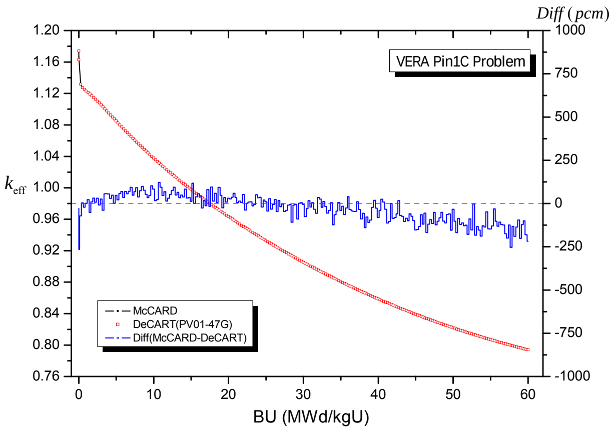

Fig. 2. Comparison of the evolutions of infinite multiplication factor and their discrepancies over burnup for VERA pin problem (242 DTS)

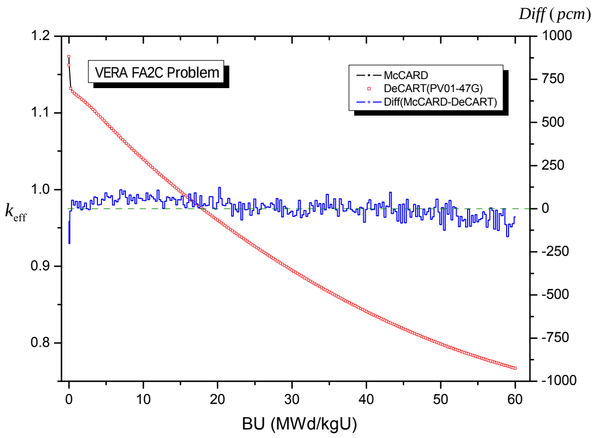

Fig. 3. Comparison of the evolutions of infinite multiplication factor and their discrepancies over burnup for VERA FA problem (242 DTS)

In particular, to confirm the sensitivity due to the burnup interval, MC depletion analyses having a different DTS were performed. Figure 4 presents the detail description of three burnup interval cases: 40, 123, and 242 DTS. Table I shows a comparison of k_{inf} calculated by McCARD for each DTS case. At the end of the burnup, the difference in k_{inf} between the 242 and 40 DTS is 347 pcm, while that between the 242 and 123 DTS is 55 pcm. It should be noted that the MC depletion results depend on how to split the burnup interval. However, it is observed that there are no significant differences between the DeCART results as show in Table 2.

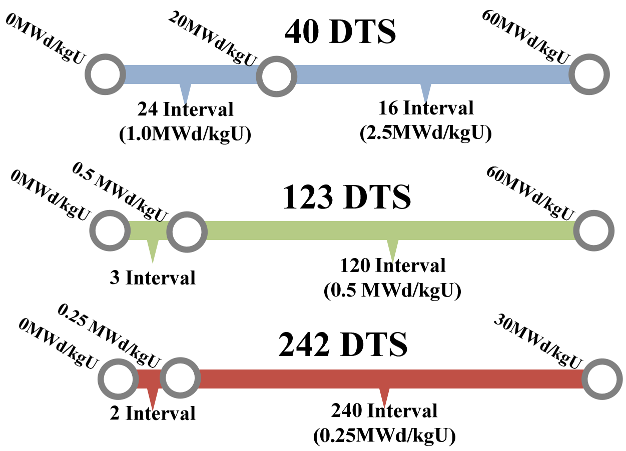

Fig. 4. Description of each burnup interval case

Table 1: Comparison of the infinite multiplication factors due to burnup intervals (Pin1C problem)

Burnup (MWd/kgU)	McCARD (242DTS)			
	k_{inf}	SD*	$\Delta\rho^{**}$ (123DTS)	$\Delta\rho^{***}$ (40 DTS)
0.0	1.17432	27	0	0
0.5	1.12762	29	-15	-25
1.0	1.12326	29	-26	5
5.0	1.08549	26	-86	-65
10.0	1.03829	28	-131	-77
20.0	0.96491	27	-187	-47
30.0	0.90665	27	-151	23
40.0	0.86053	26	-173	130
50.0	0.82335	26	-182	98
60.0	0.79559	25	-55	347

* SD(Standard Deviation) = $1 \cdot \sigma$
** $\Delta\rho = (1/k_{\infty}^{40DTS} - 1/k_{\infty}^{123DTS}) \times 10^5$
*** $\Delta\rho = (1/k_{\infty}^{64DTS} - 1/k_{\infty}^{123DTS}) \times 10^5$

Table 2: Comparison of the infinite multiplication factors due to burnup intervals (Pin1C problem)

Burnup (MWd/kgU)	DeCART (242DTS)		
	$k_{\inf}$	$\Delta\rho^{*}$ (123DTS)	$\Delta\rho^{**}$ (40 DTS)
0.0	1.17393	0	0
0.5	1.12747	0	0
1.0	1.12295	-2	-2
5.0	1.08503	-1	1
10.0	1.03778	0	2
20.0	0.96345	0	2
30.0	0.90536	1	-4
40.0	0.85865	1	4
50.0	0.82190	1	12
60.0	0.79387	3	22

* $\Delta\rho = (1/k_{\infty}^{40DTS} - 1/k_{\infty}^{123DTS}) \times 10^5$
** $\Delta\rho = (1/k_{\infty}^{64DTS} - 1/k_{\infty}^{123DTS}) \times 10^5$

2.3 Uncertainty Propagation Analysis in VERA MC Depletion Calculations by S/U and S. S. method

In the previous section, it was observed that there are significant differences in the MC depletion results owing to the burnup interval. First, to find out the source of the error, stochastic uncertainty propagation analyses were performed in MC depletion calculations. There are two approaches for an uncertainty propagation analysis. One is a sensitivity and uncertainty (S/U) analysis method based on MC perturbation techniques, whereas the other is stochastic sampling (S. S.) or a brute force method by sampling the input parameters according to their uncertainties. In this work, the SNU formulation [6] aimed at quantifying uncertainties in the Monte Carlo (MC) tallies as well as the nuclide number density estimates in an MC depletion analysis is used to conduct an uncertainty propagation analysis through the S/U approach. Meanwhile, the S. S. method is based on the replica calculations with different random number sequences. Figure 5 presents the algorithm and flows of the uncertainty propagation procedure by the SNU formulation.
For the uncertainty propagation analyses, all MC runs at each DTS were conducted based on 150 cycles including 50 inactive cycles with 10,000 particle histories per cycle, assuming that the number densities for only six actinide nuclides - U^{235}, U^{238}, Pu^{239}, Pu^{240}, Pu^{241}, Pu^{242} have their uncertainties. For burnup interval condition, 40 DTS was used. Table 3 shows the uncertainty of $k_{\inf}$ calculated by the SNU formulation. Eq. 1 shows that the variance of $k_{\inf}$ arises from the four sources.

$$\sigma^2[k_{\inf}] = \sigma_{STATS}^2 + \sigma_{XX}^2 + \sigma_{NN}^2 + 2\sigma_{NX}^2 \qquad \dots (1)$$

where $\sigma_{XX}^2 = \sum_{i,\alpha,g}\sum_{i',\alpha',g'} \rho[\sigma_{\alpha,g}^i, \sigma_{\alpha',g'}^i] \times \delta k_{\inf}(\sigma_{\alpha,g}^i) \times \delta k_{\inf}(\sigma_{\alpha',g'}^i),$

$$\sigma_{NN}^2 = \sum_{m,i}\sum_{m',i'} \rho[N_{m,i}^n, N_{m',i'}^n] \times \delta k_{\inf}(N_{m,i}^n) \times \delta k_{\inf}(N_{m',i'}^n),$$

and

$$\sigma_{NX}^2 = \sum_{m,i}\sum_{i',\alpha',g'} \rho[N_{m,i}^n, \sigma_{\alpha',g'}^i] \times \delta k_{\inf}(N_{m,i}^n) \times \delta k_{\inf}(\sigma_{\alpha',g'}^i).$$

$N_{m,i}^n$ is the number density of nuclide i in cell m at DTS n whereas $\sigma_{\alpha',g'}^{i'}$ is the α'-type cross section of nuclide i' for the group g' neutrons. Note that $\sigma_S^2[k_{\inf}]$ is uncertainty that comes from the statistical uncertainty in the MC simulations. $\sigma_{NN}^2[k_{\inf}]$ and $\sigma_{XX}^2[k_{\inf}]$ come from uncertainties of nuclide number densities and microscopic cross sections, respectively, whereas $2\sigma_{NX}^2[k_{\inf}]$ comes from the cross correlation between them. In this work, the covariance matrix of cross sections provided from the evaluated nuclear data library was not used because it was focused only on statistical errors. Therefore, $\sigma_{XX} = 0$ and $\sigma_{NX} = 0$. Overall, it was observed that the $\sigma_S[k_{\inf}]$ arising from the unalloyed statistical uncertainty at each DTS is dominant.

In the S. S. method [7], one can formally define the mean value, $\overline{k_{\inf}}$, and variance, $\sigma^2(k_{\inf})$, as below:

$$\overline{k_{\inf}} \cong \frac{1}{N}\sum_{i=1}^{N} k_{\inf}^i \qquad \dots (2)$$

$$\sigma^2(k_{\inf}) \cong \frac{1}{N-1}\sum_{i=1}^{N}(k_{\inf}^i - \overline{k_{\inf}})^2. \qquad \dots (3)$$

where $k_{\inf}^i$ is the infinite multiplication factor calculated by the i-th sample using 10,000 particle histories per cycle and 100 active cycles. Additionally, for the comparison, $k_{\inf}^{REF}$ is calculated with 10,000 particle histories per cycle and 500 active cycles. Table 4 shows the uncertainty of $k_{\inf}$ calculated by the S. S. method. The uncertainty was estimated from 60 replicas with a different random number of sequences. It was observed that the uncertainties estimated by the S. S. method are similar to those by the S/U method. In view of the results thus far achieved, it is explained that the effect by the stochastic uncertainty propagation did not make much difference in $k_{\inf}$ during the MC depletion analysis due to the burnup interval.

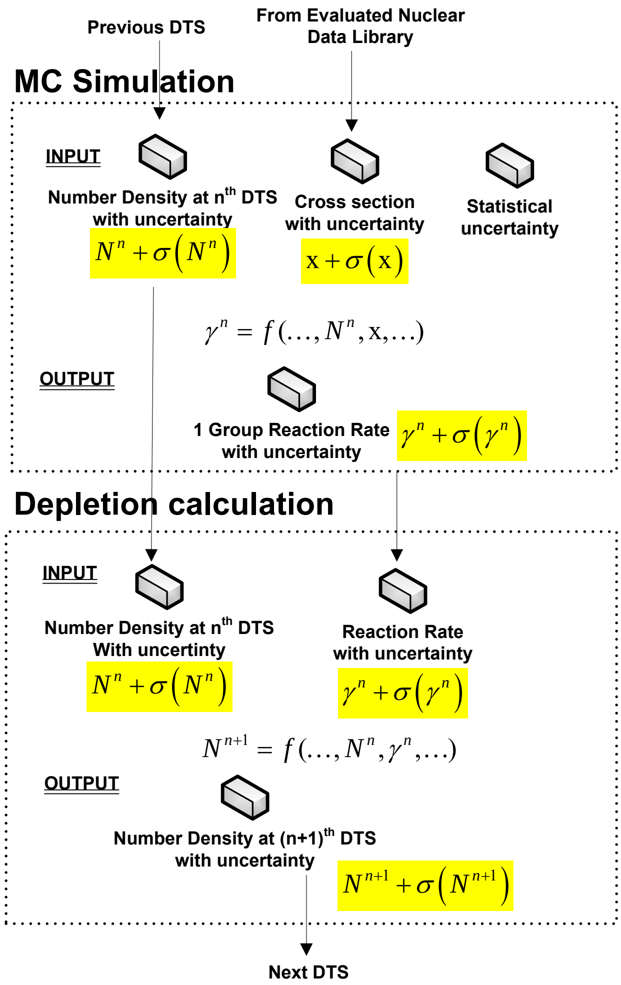

Fig. 5. Flowchart of uncertainty propagation procedure in MC depletion analysis by the SNU formulation

Table 3: Uncertainty of the infinite multiplication factors by SNU formulations (40 DTS)

Burnup (MWd/kgU)	Uncertainty of infinite multiplication factor			
	$\sigma[k_{\inf}]$	σ_{STATS}	σ_{NN}	σ_{XX}
0	0.00090	0.00090	0.00000	
0.5	0.00095	0.00095	0.00001	
1	0.00072	0.00072	0.00001	
5	0.00095	0.00095	0.00005	
10	0.00081	0.00081	0.00007	
20	0.00080	0.00079	0.00010	-
30	0.00081	0.00079	0.00020	
40	0.00073	0.00069	0.00023	
50	0.00067	0.00062	0.00026	
60	0.00074	0.00069	0.00027	

Table 4: Uncertainty of the infinite multiplication factors by stochastic sampling method (40 DTS)

Burnup (MWd/kgU)	Infinite multiplication factor and its uncertainty		
	$k_{\inf}^{REF}$ *	$\overline{k_{\inf}}$	$\sigma^2(k_{\inf})$
0	1.17432	1.17469	0.00070
0.5	1.12775	1.12765	0.00058
1	1.12287	1.12319	0.00060
5	1.08525	1.08523	0.00064
10	1.03771	1.03804	0.00053
20	0.96361	0.96381	0.00062
30	0.90522	0.90518	0.00057
40	0.85829	0.85803	0.00063
50	0.82146	0.82108	0.00065
60	0.79305	0.79282	0.00079

* $k_{\inf}$ of single MC run by 10,000 particle/cycle and 500 active cycle

In addition, the SNU formulation can facilitate the estimation of the number density uncertainties at each DTS. Eq. 4 shows that the variance of the number density arises from the two sources – number densities and one-group reaction rates.

$$\sigma^2[N_{m,i}^{n+1}] = \sigma_{NN}^2 + \sigma_{RR}^2 + 2\sigma_{NR}^2 \qquad \ldots (4)$$

where $\sigma_{RR}^2 = \sum_{j,\alpha}\sum_{j',\alpha'} \rho[r_{\alpha,m}^{j,n}, r_{\alpha',m}^{j',n}] \times \delta N_{m,i}^{n+1}(r_{\alpha,m}^{j,n}) \times \delta N_{m,i}^{n+1}(r_{\alpha',m}^{j',n}),$

$$\sigma_{NN}^2 = \sum_{i'}\sum_{i"} \rho[N_{m,i'}^{n}, N_{m,i"}^{n}] \times \delta N_{m,i}^{n+1}(N_{m,i'}^{n}) \times \delta N_{m,i}^{n+1}(N_{m,i"}^{n}),$$

and

$$\sigma_{NR}^2 = \sum_{j,\alpha}\sum_{i"} \rho[r_{\alpha,m}^{j,n}, N_{m,i"}^{n}] \times \delta N_{m,i}^{n+1}(r_{\alpha,m}^{j,n}) \times \delta N_{m,i}^{n+1}(N_{m,i"}^{n}).$$

$r_{\alpha,m}^{j,n}$ is the α-type microscopic reaction rate of nuclide j for the region m at DTS n. Table 5 and 6 present the uncertainties of the U^{235} and Pu^{239} number density by S. S. and S/U method, respectively. Similarly for the uncertainty of the infinite multiplication factor, $\sigma[N_{m,i}^{n+1}]$ by S. S. method is in good agreement with one by the S/U method. At 60MWd/kgU, the relative uncertainty, $\sigma[N_{m,i}^{n+1}]/N_{m,i}^{n+1}$, of U^{235} number density is about 0.09% while that of Pu^{239} number density is about 0.11%.

Table 5: Uncertainty of the U^{235} number density by stochastic sampling and S/U method (40DTS)

Burnup (MWd/kgU)	Uncertainty of U^{235} number density			
	S.S. Method	S/U Method*		
	$\sigma[N_{m,i}^{n+1}]$	$\sigma[N_{m,i}^{n+1}]$	σ_{NN}	σ_{RR}
0	-	-	-	-
0.5	3.26E-09	9.99E-09	6.78E-09	7.30E-09
1	6.22E-09	1.78E-08	9.80E-09	1.48E-08
5	2.35E-08	4.95E-08	4.30E-08	2.20E-08
10	2.56E-08	6.67E-08	6.22E-08	1.90E-08
20	4.15E-08	7.81E-08	7.51E-08	1.39E-08
30	4.70E-08	8.84E-08	7.89E-08	2.95E-08
40	5.51E-08	8.44E-08	7.81E-08	2.05E-08
50	6.14E-08	7.47E-08	7.03E-08	1.43E-08
60	5.30E-08	6.14E-08	5.86E-08	9.40E-09

* Used the notations from Eq.(4).

Table 6: Uncertainty of the Pu^{239} number density by stochastic sampling and S/U method (40DTS)

Burnup (MWd/kgU)	Uncertainty of Pu^{239} number density			
	S.S. Method	S/U Method*		
	$\sigma[N_{m,i}^{n+1}]$	$\sigma[N_{m,i}^{n+1}]$	σ_{NN}	σ_{RR}
0	-	-	-	-
0.5	5.55E-09	3.25E-09	2.10E-09	2.48E-09
1	1.01E-08	7.16E-09	3.04E-09	6.49E-09
5	3.74E-08	2.88E-08	2.32E-08	1.66E-08
10	3.85E-08	4.15E-08	3.45E-08	2.13E-08
20	6.71E-08	5.89E-08	5.13E-08	2.44E-08
30	1.22E-07	1.12E-07	7.89E-08	6.88E-08
40	1.32E-07	1.42E-07	1.03E-07	8.14E-08
50	1.44E-07	1.55E-07	1.14E-07	8.43E-08
60	1.69E-07	1.64E-07	1.21E-07	8.69E-08

* Used the notations from Eq.(4).

2.4 Behavior of Reaction Rate and Number Density

Table 7 presents the number densities of major actinide isotopes at 60 MWd/kgU and the difference in the number density between 242 DTS and 40 DTS. Table 8 shows the number densities of U^{235} over burnup for VERA pin depletion benchmark by McCARD. The difference in U^{235} number density between 242 DTS and 40 DTS increases to about 1.4% with burnup. The difference leads to the difference in k_{inf} as shown in Table 1. Because the number densities for each isotope are the solutions of the depletion chain equations, the precious one-group microscopic reaction rate or cross section must be calculated for the prediction of the precious number density. Table 9 indicates the one-group cross section of U^{235}, which will be used to solve the depletion equations. It should be noted that the one-group cross sections or microscopic reaction rates decrease non-linearly over a burnup. Because of the non-linearity, the use of the predictor method or the coarse burnup interval may cause the error for the MC depletion results.

Table 7: Number density for major actinide isotope at 60 MWd/kgU by McCARD

Isotope	Number Density (#/cm/barn)		
	242 DTS	40 DTS	*Diff* (%)*
U-235	7.291E-05	7.189E-05	-1.39
U-238	2.104E-02	2.104E-02	-0.01
Pu-239	1.513E-04	1.490E-04	-1.55
Pu-240	7.528E-05	7.534E-05	0.09
Pu-241	4.847E-05	4.840E-05	-0.15
Pu-242	2.808E-05	2.836E-05	1.01
Am-241	1.409E-06	1.399E-06	-0.68
Cm-244	6.409E-06	6.479E-06	1.09

$*Diff = (N^{40DTS} - N^{242DTS}) / N^{242DTS} \times 100$

Table 8: Number density of U^{235} over burnup for VERA pin depletion benchmark by McCARD

Burnup (MWD/kgU)	Number Density of U-235 (#/cm/barn)		
	242 DTS	40 DTS	*Diff* (%)*
0.0	7.181E-04	7.181E-04	-
0.5	7.046E-04	7.046E-04	0.01
1.0	6.914E-04	6.913E-04	-0.01
5.0	5.970E-04	5.968E-04	-0.03
10.0	4.989E-04	4.986E-04	-0.06
20.0	3.479E-04	3.472E-04	-0.19
30.0	2.398E-04	2.389E-04	-0.35
40.0	1.630E-04	1.619E-04	-0.63
50.0	1.094E-04	1.083E-04	-0.98
60.0	7.291E-05	7.189E-05	-1.39

$*Diff = (N^{40DTS} - N^{242DTS}) / N^{242DTS} \times 100$

Table 9: One-group cross section of U^{235} for burnup

Burnup (MWD/kgU)	One-group Cross section of U^{235} (barn)		
	242 DTS	40 DTS	*Diff* (%)*
0.0	5.970E+01	5.970E+01	-
0.5	5.762E+01	5.766E+01	0.07
1.0	5.698E+01	5.701E+01	0.06
5.0	5.332E+01	5.338E+01	0.11
10.0	5.072E+01	5.084E+01	0.22
20.0	4.819E+01	4.838E+01	0.40
30.0	4.692E+01	4.714E+01	0.47
40.0	4.604E+01	4.631E+01	0.57
50.0	4.530E+01	4.558E+01	0.61
60.0	4.460E+01	4.485E+01	0.57

$*Diff = (\sigma^{40DTS} - \sigma^{242DTS}) / \sigma^{242DTS} \times 100$

$**\sigma = one\ group\ cross\ section \equiv (\sigma\phi)/\phi$

3. Conclusions

It is still expensive and challenging to perform a depletion analysis by a MC code. Nevertheless, many studies and works for a MC depletion analysis have been conducted to utilize the benefits of the MC method. In this study, McCARD MC and DeCART MOC transport calculations are performed for the VERA pin and FA depletion benchmarks. The DeCART depletion calculations are conducted to examine the depletion capability of the newly generated multi-group cross section library. The DeCART depletion calculations give excellent agreement with the McCARD reference one.

From the McCARD results, it is observed that the MC depletion results depend on how to split the burnup interval. On the other hand, there are insignificant differences between the DeCART results by the three burnup interval conditions as shown in Table 2. First, only to quantify the effect of the stochastic uncertainty propagation at 40 DTS, the uncertainty propagation analyses are performed using the S/U and S.S. method. From the results shown in Table 3 and 4, the fact that the final propagated uncertainty of k_{inf} is similar to the unalloyed statistical uncertainty over the whole depletion range indicates that the exclusive effect only by stochastic uncertainty propagation is not significantly large. Second, the behavior of the number density and microscopic reaction rate over the burnup are observed as shown in Tables 7 through 9. It should be noted that the one-group cross sections or microscopic reaction rates decrease non-linearly over burnup. Under these circumstances, the burnup interval in the MC depletion analysis must be sufficiently fine to reduce the uncertainty of the MC solutions at each DTS and obtain the accurate number densities.

Generally, it is well known that the fine burnup interval for a Gd-bearing pin or FA depletion analysis is needed to predict the accurate number densities of Gd isotopes [8]. Consequently, it was concluded that the proper fine burnup interval should be used to obtain the accurate MC results in a MC depletion analysis even if there is no burnable absorber in the nuclear system.

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