# Multi-Group Library Generation with Explicit Resonance Interference Using Continuous Energy Monte Carlo Calculation

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## 1. Introduction

Various multi-group transport codes have been developed and widely used in a nuclear core design analysis such as a lattice calculation or a whole core calculation. [1,2,3] KAERI (Korea Atomic Energy Research Institute) has developed the transport lattice code KARMA (Kernel Analyzer by Ray-tracing Method for fuel Assembly) [4] and DeCART (Deterministic Core Analysis based on Ray Tracing) [5] for a multi-group neutron transport analysis of light water reactors (LWRs). These codes adopt the method of characteristics (MOC) to solve the multi-group transport equation and resonance fixed source problem, the subgroup and the direct iteration method with resonance integral tables [6] for resonance treatment.

With the development of the DeCART and KARMA code, KAERI has established its own library generation system for a multi-group transport calculation. In the KAERI library generation system, the multi-group average cross section and resonance integral (RI) table are generated and edited using PENDF (point-wise ENDF) and GENDF (group-wise ENDF) produced by the NJOY code [7]. Conventionally, the RI tables are calculated by solving the slowing-down equations for a heterogeneous system with PENDF through a deterministic method. In a previous study [8], another approach obtaining RI tables or effective cross sections was applied using a Monte Carlo (MC) calculation. The new approach is simple and effective because the MC method can handle a continuous energy cross section library in ACE format and a complex geometry information, easily.

In this study, a multi-group cross section library for the transport codes was generated using a new procedure for the resonance treatment with an explicit resonance interference. The RI tables for $U^{235}$ and $U^{238}$ were calculated by the McCARD code [9] while those for other isotopes were calculated by a conventional procedure. Lastly, to verify the new procedure and examine a new cross section library, various benchmark calculations were performed and the results compared with the reference solutions.

## 2. Methods for Multi-group Library Generation

### *2.1 KAERI Library Generation System [10]*

Figure 1 shows a flowchart of the KAERI library generation system. Multi-group microscopic cross sections for all of the nuclides are processed using various modules of the NJOY code. The PENDF file by the BROADR module and the GENDF output file by the GROUPR module are generated and used in a multi-group average cross section and resonance integral table generation, respectively. For user friendliness, the ANJOY and ANJOYG codes automatically prepare NJOY inputs and batch files for all nuclides and the temperatures defined in the user's input files. The GENDF output files are edited and reformulated by GREDIT to be used in the transport code. Meanwhile, the GAMINR module of the NJOY code produced the photo-atomic GENDF output files for gamma library generation. MERIT generates the hydrogen equivalent intermediate resonance parameters and the RI tables as a function of the background cross section and temperature only for resonant nuclides defined by the user's input. As the next step, the SUBDATA generates the sub-group data including the subgroup levels and their corresponding weights such that the RIs reconstructed with these subgroup data approximate accurately the original RIs produced by MERIT. Finally, the LIBGEN generates the ASCII formatted multi-group cross section library which can be used in the transport lattice code by assembling the output files of GREDIT, GREDITG and SUBDATA, and the additional data such as the decay and fission product yield data for a burnup analysis. The LIBGEN provides a group collapsing procedure with the given neutron spectra. The ASCII formatted multi-group cross section library is converted into a binary library through the LIBFORM.

In this study, a new procedure for the RI table generation using MC calculations is applied. The MIG code [11] generates McCARD inputs for various background cross sections that are prepared by changing the region volumes and atomic number densities, and a batch file for the automatic calculations. M2M and EDIT_XS convert the output of McCARD

into an external input used in the MERIT code. Naturally, the multi-group average cross section calculated by McCARD can be used as the input of the LIBGEN code.

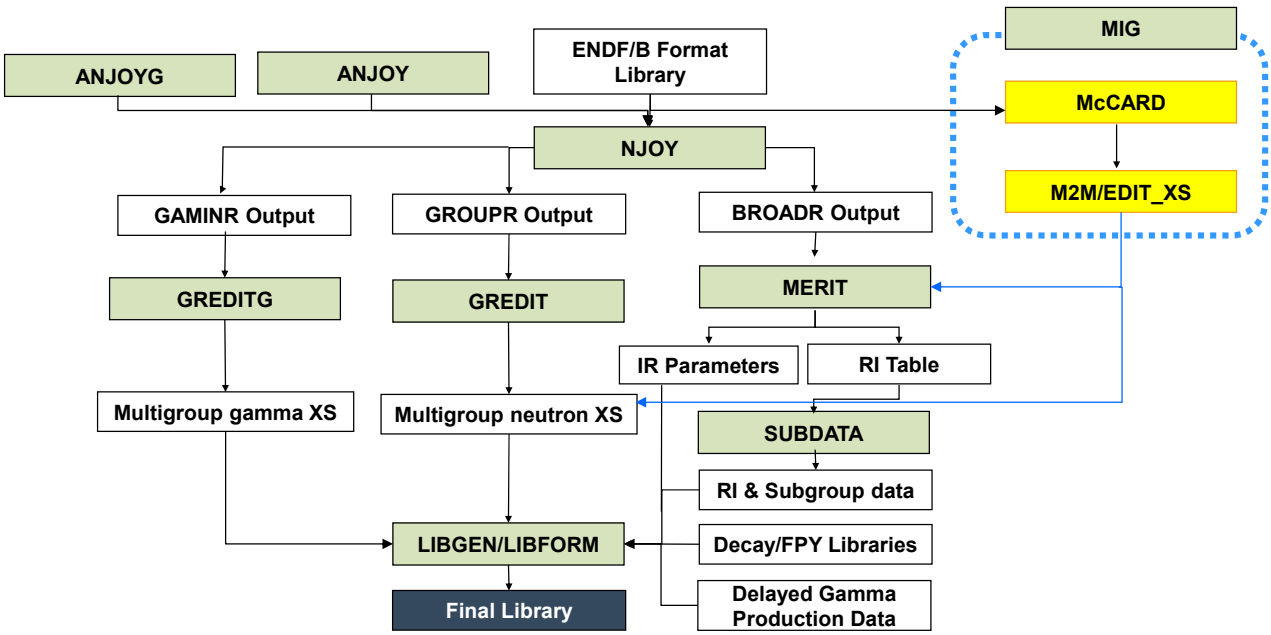


Fig. 1. Flowchart of KAERI cross section library generation system

### *2.2 Multi-group Cross Section Generation with Realistic Spectrum Weight*

The accuracy of the group-average cross section is determined by the group structure and the weight function. While taking a finer energy group structure will reduce the uncertainty of the cross section, it increases the cost in terms of time and memory. In general, the weight function - flux energy spectrum for the GENDF generation is not known. In the GROUPR module of NJOY code, a typical built-in flux spectrum was provided with various IWT options. The weight function option IWT=4, which was used in the conventional procedure, provided a Maxwellian distribution at thermal energy, a 1/E function at intermediate energy, and a fission spectrum at high energy. To read the spectrum of the realistic system, IWR=1 option is used. In the new procedure, the 1900-group typical PWR FA spectrum calculated by the McCARD code is used for the GENDF processing.

### *2.3 Correction of Effective Fission Product Yield*

An ENDF/B decay data file such as ENDF-349 [12] provides the fission-product yield (FPY), which is the probability of formation in fission of all stable nuclides of a given mass number. ENDF/B decay data includes FPY for the nuclides that undergo fission by neutrons at several energies – thermal energy (T), fission spectrum energy (F), 14MeV high energy (H or He), and spontaneous fission (S). In the old library, we selected the FPY at the only lowest energy points (T) for simplicity. In the new KAERI library generation system, the LIBGEN code reads FPY data from the ENDF/B FPY data and obtain the effective FPY using fission reaction rates which can be given through the user's input or transport code calculation. The effective FPY can be calculated by

$$f_{ik}^{eff}(t) = \frac{\sum_{g=1}^{G} f_{ik}^{g} \cdot \sigma_{f,g}^{i}\phi_g(t)}{\sum_{g=1}^{G} \sigma_{f,g}^{i}\phi_g(t)}. \qquad \text{.....(1)}$$

where $\sigma_{f,g}^{i}\phi_g(t)$ is the $g$-th group fission reaction rate of $i$ isotope at depletion time $t$ while $f_{ik}^{g}$ indicates the $g$-th group yield for a $k$ fission product isotope produced by the fission of an $i$ isotope. In general, the FPYs at three energy group – thermal, fission spectrum, and 14 MeV high energy are provided.

### *2.4 Resonance Treatment for All FP Nuclides*

In a previous study, it was observed that an error in the cross section of some FP and actinides is one of the sources for the large discrepancy between k-effectives due to burnup. In order to reduce the error in the cross section, most of fission product nuclides are processed as resonant nuclides. As the attribute of the fission product nuclides changes, the definition of the resonant

nuclide in the multi-group transport code is modified. The number of resonant nuclides for a fission product is increased from 51 to 131 whereas that for actinide is increased from 11 to 29. Therefore, the total number of all resonant nuclides is increased from 62 to 160.

## 3. Result for PWR Benchmark Problem

### *3.1 DeCART Multi-group Library Generation for PWR system*

The new multi-group libraries for the DeCART code are generated through several sequential steps as shown in Fig 1. Table I shows the detailed condition for each library generation. In the new library, two neutron/gamma coupled cross section libraries having different energy group structures from each other are generated using ENDF/B-VII.1 evaluated nuclear data library: 47 group neutron/18 group gamma, 190 group neutron/48 group gamma. The adopted energy group structures are the same as those used in HELIOS. PV01-190G and PV01-47G are the multi-group cross section libraries generated using the new library generation system with two different energy group structure. The RI tables for $U^{235}$ and $U^{238}$ are calculated by the MC calculations. The RI table generation procedures for the other isotopes are the same as those used in a conventional procedure. For comparison, PV00-190G is generated using all options used in a conventional procedure except the $U^{238}$ absorption cross section adjustment.

Table I: Description of DeCART Library for PWR Benchmark Calculation

| Case | PV00-190G | PV01-190G | PV01-47G |
|---|---|---|---|
| Raw ENDL[1)] | ENDF/B-VII.1 | ENDF/B-VII.1 | ENDF/B-VII.1 |
| Group Structure (Neutron/Gamma) | 190g/48g | 190g/48g | 47g/18g |
| NJOY weight function (IWT) | 4 | 1 | 1 |
| RIT Generaiton by MC Cal. [2)] | None | $U^{235}$ & $U^{238}$ | $U^{235}$ & $U^{238}$ |
| Effective FPY | None | Yes | Yes |
| Num.of Resonant Nuc. [3)] | 62 | 160 | 160 |

1) Evaluated Nuclear Data Library
2) Resonance Integral Tables Generation by McCARD calculations
3) The total number of the resonant nuclides

### *3.2 Verification of New DeCART Multi-group Library*

To verify the newly generated libraries, the pin-cell problems are considered. The pin problem is a pin cell problem which represents a typical PWR pin cell, that is the same as that used in RI table generation. Figure 2 shows the configuration of the pin-cell problem. The pin pitch is 1.2882 cm whereas the radius of 4 w/o enriched $UO_2$ fuel region is 0.4025 cm. The radius of the aluminum cladding region is 0.4759 cm. In all DeCART calculations, the direct iteration method with a resonance integral table is used for a resonance treatment. Since the resonance interference is already considered in the generation of the RI table for $U^{235}$ and $U^{238}$, the resonance interference procedure was turned off in the transport code.

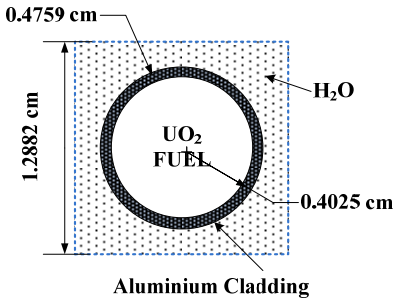


Fig. 2. Configuration of Pin Cell Problem

Table II shows the k-effectives calculated by the DeCART code for the pin-cell benchmark and a comparison with the McCARD reference solutions. The k-effective by PV01-190G and PV01-47G is closer to the reference than PV00-190G. The maximum error of PV01-47G is 66 pcm, whereas that of PV00-190G is 651 pcm. There are considerable differences between PV00-190G and the reference because the $U^{238}$ absorption cross section adjustment is excluded from the conventional procedure.

Table II : *k*-effectives for 4 w/o PWR pin-cell problems

| Temp. [1)] (kelvin) | $k_{eff}$ [2)] (Ref.) | $\Delta\rho$ [3)] | | |
|---|---|---|---|---|
| | | PV00-190G | PV01-190G | PV01-47G |
| 300 | 1.38932 | 288 | -22 | -51 |
| 500 | 1.37841 | 328 | -6 | -4 |
| 700 | 1.36954 | 363 | 3 | 11 |
| 1100 | 1.35587 | 484 | 19 | 66 |
| 2000 | 1.33076 | 651 | 42 | 23 |

1) Temperature in unit of kelvin.
2) The k-effectives calculated by McCARD ( $\sigma(k_{eff}) < 10$ pcm ).
3) $\Delta\rho = \left(1/k_{\text{eff}}^{DeCART} - 1/k_{\text{eff}}^{McCARD}\right) \times 10^5$ .

Figures 3-5 provide a comparison of the self-shielded absorption and fission cross section for $U^{235}$ and $U^{238}$ at 300K. For the comparison, the quantitative analysis for the reactivity difference between McCARD and DeCART is performed. Absorption section differences between McCARD and DeCART for the *i* istope and energy group *g'* are converted into the reactivity differences in pcm for each group using Eq. (2). A cap

(^) indicates data from the DeCART while no-cap indicates data from McCARD. *k* denotes fissionable nuclides such as $U^{235}$ and $U^{238}$. The other notation is standard. As shown in Figs. 3-5, the absorption and fission cross sections of PV00-190G, obtained from the conventional method, show a significant difference. On the other hand, those of PV01-190G from the new method are in good agreement with the reference.

$$\Delta\rho^{i}_{a,g'} = \left[ \frac{1}{k_\infty} - \frac{\sum_{g,k} N_k \sigma_{a,g,k}\phi_g - N^i \phi_{g'}\left(\sigma^i_{a,g'} - \hat{\sigma}^i_{a,g'}\right)}{\sum_{g,k} N_k \nu\sigma_{f,g,k}\phi_g} \right] \times 10^5, \quad \text{..... (2)}$$

$$\text{where } k_\infty = \frac{\sum_{g,k} N_k \nu\sigma_{f,g,k}\phi_g}{\sum_{g,k} N_k \sigma_{a,g,k}\phi_g},$$

In view of the results thus far achieved, it was verified that the DeCART calculations can reproduce the McCARD RI calculations exactly for the same problem, and that the new method works reasonably well.

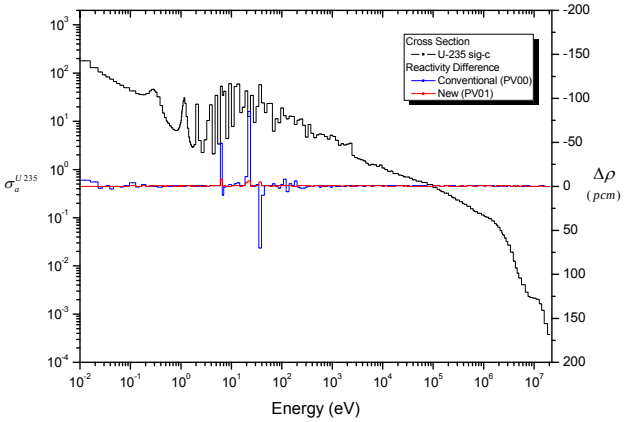


Fig. 3. Comparison of the multi-group absorption cross section of $U^{235}$ at 300K

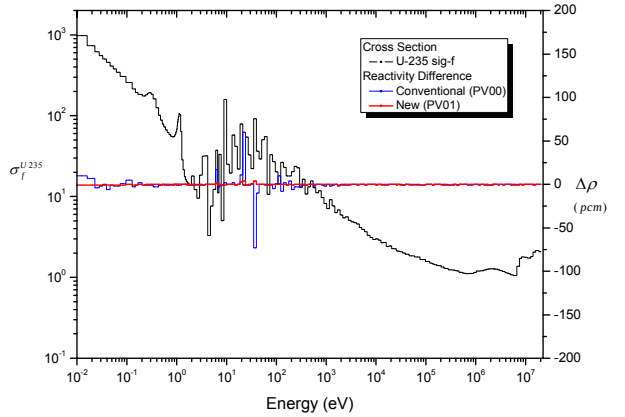


Fig. 4. Comparison of the multi-group fission cross section of $U^{235}$ at 300K

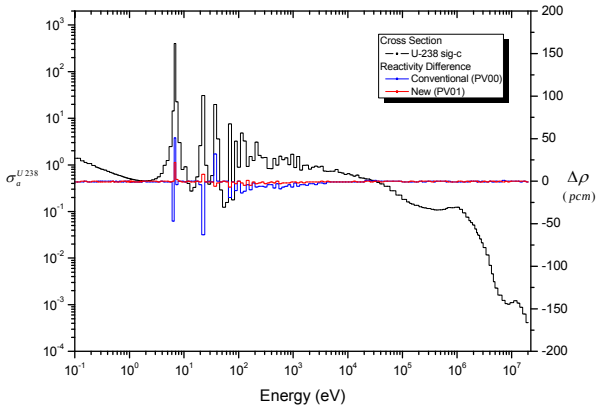


Fig. 5 Comparison of the multi-group absorption cross section of $U^{238}$ at 300K

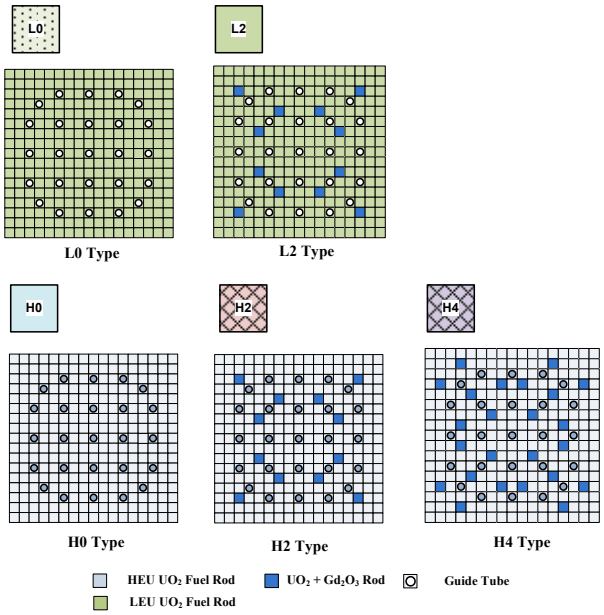


Fig. 6. Configuration of Fuel Assembly Problem

Table III compares the k-effectives for typical PWR FA problems as shown in Fig. 6. Similar to the results of the pin-cell benchmark, the PV01-190G and PV01-47G agree well with the reference solutions.

Table III : *k*-effectives for PWR FA problem (600K)

| FA. | $k_{eff}$ [1] (reference) | $\Delta\rho$ [2] | | |
|---|---|---|---|---|
| | | PV00-190G | PV01-190G | PV01-47G |
| L0 | 1.25644 | 340 | 94 | 61 |
| L2 | 1.08275 | 311 | 62 | 92 |
| H0 | 1.37876 | 314 | -96 | 50 |
| H2 | 1.28356 | 307 | -112 | 77 |
| H4 | 1.11525 | 252 | -168 | 97 |

1) *k*-effective calculated by McCARD ( $\sigma(k_{eff}) < 10$ pcm ).
2) $\Delta\rho = \left(1/k_{\text{eff}}^{DeCART} - 1/k_{\text{eff}}^{McCARD}\right) \times 10^5$ .

### 3.3 SMR Core Depletion Analysis

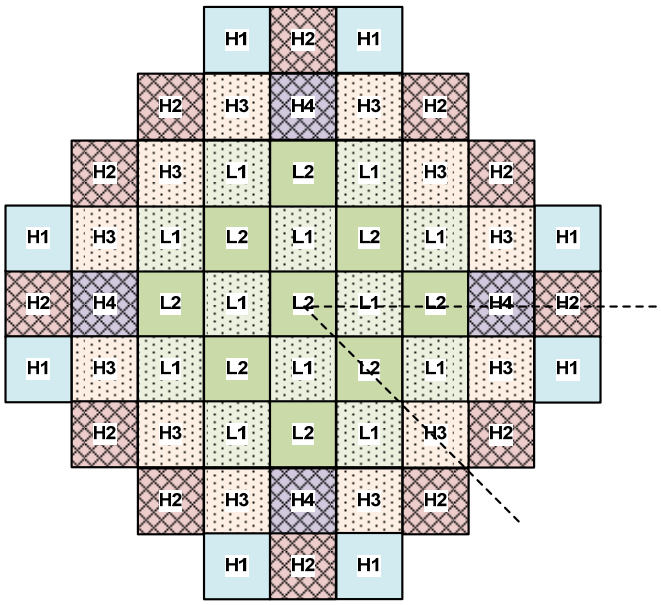


Fig. 7. Fuel Loading Pattern for 2D SMR core

To examine the new DeCART multi-group library, a depletion analyses for 2D core problem with 57 FAs for SMR (Small Modular Reactor) [13] was performed. Figure 7 shows the fuel loading pattern for the 2D SMR core. It has six types of 17x17 FAs: L1, L2, H1, H2, H3, and H4, which differ from one another in the $^{235}U$ enrichment and the number of $Gd_2O_3$-$UO_2$ fuel rods. To obtain the reference solution, the McCARD depletion analysis was performed with 20,000 neutron histories per cycle and 1,000 active cycle. For all of the calculations, T/H feedback is not considered and $P_2$ scattering cross section is used. The temperature at the fuel regions is 900K while that at the others is 600K. Figure 8 compares the k-effective of DeCART calculated by PV00-190G, PV01-47G, and the McCARD reference solution. In PV00-190G, the RMS difference is 391 pcm while the maximum difference is 580 pcm at BOC. As the core is depleted, the difference is gradually decreasing. It was noted that the error in the cross section of the FPs and actinides causes the change of the k-effective difference due to burnup. [14] In PV01-47G, generated by the new procedure, the RMS difference due to burnup is 54 pcm whereas the maximum difference is 137 pcm at about 400 EFPD. Because the number of resonant nuclides is increased for the precise cross section as explained in the previous section, the difference due to burnup is insignificant. Figure 9 shows the normalized FA-wise fission power distribution of the core at 0 EFPD and 480 EFPD. At 0 EFPD, the RMS difference between DeCART by PV01-47G and the reference is 0.25% while the maximum difference is 0.39% at Asm06_06. At 480 EFPD, the RMS difference is 0.40% while the maximum difference is 0.66% at Asm06_05. The newly generated library shows excellent performance in the core depletion problem.

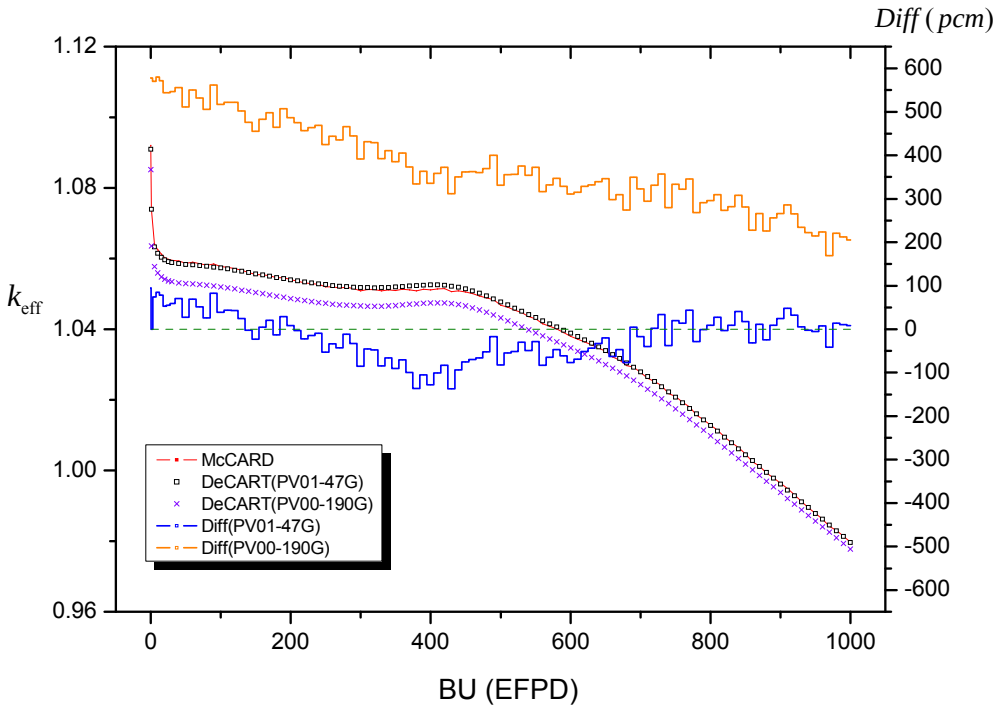


Fig. 8. Comparison of k-effective of 2D SMR core problem over burnup

**0EFPD**

| Asm05_05 | Asm06_05 | Asm07_05 | Asm08_05 | Asm09_05 | FA Name |
|---|---|---|---|---|---|
| 1.193 | 1.119 | 1.128 | 1.107 | 0.947 | McCARD |
| 1.191 | 1.119 | 1.125 | 1.109 | 0.946 | PV01-47G |
| 0.16 | 0.04 | 0.28 | -0.18 | 0.09 | Diff(%) |
| | Asm06_06 | Asm07_06 | Asm08_06 | Asm09_06 | |
| | 1.160 | 1.019 | 1.060 | 0.812 | |
| | 1.156 | 1.022 | 1.061 | 0.812 | |
| | 0.39 | -0.31 | -0.12 | 0.04 | |
| | | Asm07_07 | Asm08_07 | | |
| | | 1.069 | 0.820 | | |
| | | 1.073 | 0.818 | | RMS Diff. |
| | | -0.35 | 0.27 | | 0.25 |

**480 EFPD**

| Asm05_05 | Asm06_05 | Asm07_05 | Asm08_05 | Asm09_05 | FA Name |
|---|---|---|---|---|---|
| 1.167 | 1.178 | 1.144 | 1.156 | 0.829 | McCARD |
| 1.174 | 1.170 | 1.144 | 1.159 | 0.828 | PV01-47G |
| -0.59 | 0.66 | -0.01 | -0.18 | 0.18 | Diff(%) |
| | Asm06_06 | Asm07_06 | Asm08_06 | Asm09_06 | |
| | 1.165 | 1.107 | 1.075 | 0.706 | |
| | 1.161 | 1.111 | 1.080 | 0.704 | |
| | 0.32 | -0.33 | -0.45 | 0.23 | |
| | | Asm07_07 | Asm08_07 | | |
| | | 1.123 | 0.794 | | |
| | | 1.123 | 0.791 | | RMS Diff. |
| | | -0.05 | 0.32 | | 0.40 |

Fig. 9. Comparison of FA-wise power distribution of 2D SMR core (PV01-47G)

## 3. Conclusions

In this study, multi-group cross section libraries for the DeCART code were generated using a new procedure. The new procedure includes generating the RI tables based on the MC calculations, correcting the effective fission product yield calculations, and considering most of the fission products as resonant nuclides.

Since the resonance interference formula in the subgroup and the direct resonance integral method are still incomplete [15], the conventional method requires an adjustment procedure - the $U^{238}$ absorption cross section adjustment. The new method does not need additional processing because the MC method can handle any geometry information and material composition. In this study, the new method is applied to the dominant resonance nuclide such as $U^{235}$ and $U^{238}$ and the conventional method is applied to the minor resonance nuclides.

To examine the newly generated multi-group cross section libraries, various benchmark calculations such as pin-cell, FA, and core depletion problem are performed and the results are compared with the reference solutions. Overall, the results by the new method agree well with the reference solution. The new procedure based on the MC method were verified and provided the multi-group library that can be used in the SMR nuclear design analysis.

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