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Comparative Analysis of Group Constants using Serpent 2 and DeCART2D

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1. Introduction

Small Modular Reactors (SMRs) are attracting interest for their enhanced safety, flexibility, and economic potential. Soluble boron free (SBF) operation, an innovative feature in SMRs, offers promising advantages. However, the unique neutronics of SBF cores pose challenges for accurate analysis and design, especially in the context of regulatory validation.

In SBF SMRs, reactivity control relies solely on local elements such as control rods and burnable absorbers (BA). The increasing demand for load following operation in SMR further increases control rod movement, resulting in complex spatial and temporal variations in neutron flux and power distributions. These SBF core characteristics demand a more precise analysis code system than in the conventional reactors, both for design and regulatory validation.

Monte Carlo (MC) methods excel in modeling complex geometries and nuclear reaction, making them promising for analyzing SBF SMR cores. This study uses Serpent 2 (version 2.2,) a continuous-energy MC code for reactor physics and burnup calculations, developed by VTT Technical Research Centre of Finland [1]. However, the computational intensity of full-core MC simulations necessitates the development of hybrid approaches combining MC accuracy with deterministic nodal code speed. A critical step of these hybrid methods is the generation of accurate group constants using MC simulations.

This paper aims to generate a Serpent-based group constant generation for SBF SMR core as the first step to combine a MC code and a nodal diffusion core analysis code. The other objective is to demonstrate the accuracy of the group constants and other nodal parameters generated by DeCART2D through comparison of them against results from the well-established Monte Carlo code Serpent2. Both simulations utilize the ENDF/B-VII.1 nuclear data library for comparison. This study focuses on a representative fuel assembly (FA) design anticipated for use in SBF SMRs, featuring gadolinia burnable absorbers with 50 $^{a}/_{o}$ (atom percent) enrichment.

2. Calculation Conditions and Codes

Table I presents the FA specifications for calculation. The FA is a 17x17 Westinghouse type. The power density was calculated based on the thermal power of the i-SMR core currently under development in Korea [2]. This core has a thermal output of 520MW, contains 69 FAs, and has an axial height of 240 cm. Using these parameters, the FA power is calculated at 31.4 kW. Thus, the specific power density of 0.02527 kW/g represents the thermal output per gram of uranium (1,242 g) in this FA.

Another feature of this FA is the use of 20 UO_2-Gd_2O_3 BA rods. Gadoliniums in these BA rods have a very high neutron absorption cross-section, making it a promising material for controlling excess reactivity in SBF cores. Among the gadolinium isotopes, ^{155}Gd and ^{157}Gd have remarkably high thermal neutron absorption cross-sections $\sigma(n,\gamma)$ (^{155}Gd: 60,889 b / ^{157}Gd: 254,078 b). Enriching these isotopes can lead to more effective suppression of excess reactivity over extended fuel cycles. As shown in Table II, the combined enrichment of these two isotopes was set to 50 $^{a}/_{o}$

Table I: Target fuel FA specifications

Geometry of fuel assembly	
Power density	0.02527 kW/g
Fuel assembly array	17x17
Fuel cladding outer radius	0.4750 cm
Fuel pin pitch	1.2600 cm
Fuel pellet radius	0.4096 cm
Boron concentration	0 ppm
Number of BA pins	20
UO_2 fuel rod	
Fuel pellet density	10.209 g/cm^3
^{235}U enrichment	4.0 wt.%
UO_2-Gd_2O_3 burnable absorber rod	
Fuel pellet density	9.950 g/cm^3
^{235}U enrichment	1.8 wt. %
Gadolinium enrichment	8wt. % (^{155}Gd +^{157}Gd = 50 a/o)

Table II: Composition of the enriched gadolinium

Isotope	Abundance (%)
^{152}Gd	0.14
^{154}Gd	1.57
^{155}Gd	**24.3**
^{156}Gd	14.72
^{157}Gd	**25.7**
^{158}Gd	17.86
^{160}Gd	15.71

2.1. Serpent 2

Figure 1 shows the FA configuration modeled using Serpent 2. The FA features 24 guide tubes and 1 instrumentation tube (represented by blue circles), normal UO_2 fuel rods (orange regions), and UO_2-Gd_2O_3 BA rods (green regions). To account for radial variations in fuel composition and neutron flux during burnup calculations, the UO_2 fuel pellets were divided into 3 sub-regions, while the BA rods were segmented into 5 sub-regions. Reflective boundary conditions were applied to the assembly model.

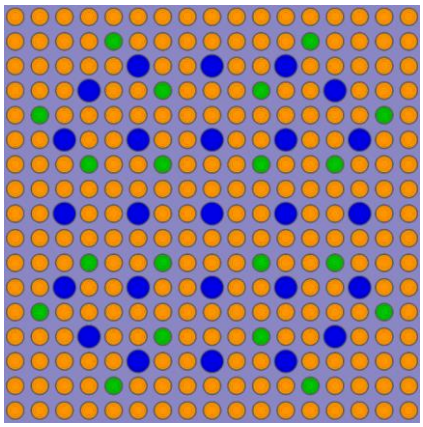

Fig.1 Configuration of FA modeled by Serpent 2

Thermal scattering data also was applied in the calculations to account for the temperature-dependent neutron interactions with light water and uranium dioxide. Specifically, the S(α,β) scattering laws for light water at 580 K (using the lwtr.25t and lwtr.26t libraries, valid for 550-600 K) and for UO_2 at 900 K (using the o2-u.25t and o2-u.26t libraries, applicable for 800-1000 K) were implemented. This approach ensures accurate modeling of neutron thermalization in the moderator and fuel materials at their respective operating temperatures. The nuclear data library ENDF/B-VII.1 was utilized for calculations. A two-group energy structure was employed for few-group constant generation, with the thermal cutoff set at 1.8554e-6 MeV (same as DeCART2D). For more detailed spectral calculations for the B_1 critical spectrum calculation, the SCALE 238-group cross-section structure was adopted as the multi-group energy grid.

2.2. DeCART2D

DeCART2D, a deterministic FA depletion code developed by KAERI (Korea Atomic Energy Research Institute), was used to generate few-group homogenized group constants (HGCs) for comparison [3]. DeCART2D solves the multi-group transport equation using the Method of Characteristics (MOC), while solving the Bateman equation through the Krylov subspace method and accounting for resonance self-shielding effects via the subgroup method. Consistently with the Serpent 2 model, the DeCART2D depletion calculations were performed with material regions divided into 3 and 5 subregions for UO_2 and UO_2-Gd_2O_3 rods, respectively. Reflective boundary conditions with octant symmetry were applied.

Ray tracing parameters were set to 0.01 cm spacing with 8 azimuthal and 4 polar angles defined in an octant angular domain. The ENDF/B-VII.1 nuclear data library was also utilized. A 47 multi-group energy structure was adopted.

3. Numerical Results and Comparison

Figure 2 shows the evolution of the infinite multiplication factor. The green line represents the DeCART2D results, while the blue line shows the Serpent2 results. The gadolinium is completely depleted at approximately 20 MWd/kg. Notably, the agreement between the two codes is remarkably close, with discrepancies remaining within a mere 50 pcm up to this point. Even after gadolinium depletion, the maximum difference only reaches about 150 pcm at around 40 MWd/kg, still indicating excellent agreement.

The Serpent 2 simulations were conducted, utilizing 260 active cycles after 100 inactive cycles, with approximately 200,000 neutrons per cycle. This resulted in a low statistical error, maintained below 9.8 pcm throughout the entire simulation.

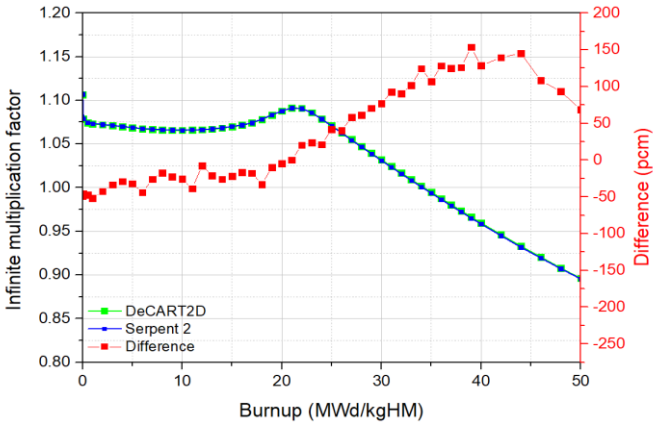

Fig.2 Comparision of the evolution of infinite multiplcation factor

Table III summarizes a comparison of homogenized 2-group constants at 20 MWd/kg between DeCART2D and Serpent codes. This table shows the various parameters for fast and thermal neutron groups, including the diffusion coefficients, the absorption cross-sections, the fission cross-sections, and the scattering matrix elements. The values calculated by both codes are shown side by side, with the rightmost column indicating the relative error between them. It's important to note that for the Serpent 2 calculations, the B_1 correction method for critical spectrum was applied. This correction is a crucial in lattice physics calculations, particularly for generating leakage-corrected few-group constants. The B_1 method is employed to address the limitations of infinite lattice calculations and to better approximate the neutron spectrum in reactor core.

Overall, the comparison demonstrates excellent agreement between DeCART2D and Serpent 2. Most parameters show relative errors well below 2.4%, with many falling under 1%. The largest discrepancies are observed in the thermal group diffusion coefficient (D_2) at 1.8255% and the upscattering cross-section ($\Sigma_{s,2->1}$) at -2.482%, but these seem to be still within acceptable errors.

Table III: Comparison of the homogenized two- group constants at 20 MWd/kgHM

Parameters		Values		**Relative error * (%)**
		DeCART	Serpent	
Fast group	$\boldsymbol{D}_1$	1.4289	1.4311	**-0.1532**
	$\boldsymbol{\Sigma}_{a,1}$	0.009569	0.009624	**-0.5839**
	$\boldsymbol{\Sigma}_{f,1}$	0.002176	0.002167	**0.4102**
	$\boldsymbol{\nu\Sigma}_{f,1}$	0.0057805	0.005757	**0.3920**
	$\boldsymbol{\kappa\Sigma}_{f,1}$	7.2375E-14	7.12E-14	**1.6161**
Thermal group	$\boldsymbol{D}_2$	0.4807	0.47195	**1.8255**
	$\boldsymbol{\Sigma}_{a,2}$	0.09958	0.09875	**0.8343**
	$\boldsymbol{\Sigma}_{f,2}$	0.05161	0.05127	**0.6494**
	$\boldsymbol{\nu\Sigma}_{f,2}$	0.1357	0.13481	**0.6587**
	$\boldsymbol{\kappa\Sigma}_{f,2}$	1.7012E-12	1.6836E-12	**1.0336**
Scattering matrix	$\boldsymbol{\Sigma}_{s,1->1}$	0.4925	4.95E-01	**-0.4125**
	$\boldsymbol{\Sigma}_{s,1->2}$	0.01686	1.68E-02	**0.1423**
	$\boldsymbol{\Sigma}_{s,2->1}$	0.0002860	0.0002931	**-2.482**
	$\boldsymbol{\Sigma}_{s,2->2}$	1.1245	1.1416	**-1.517**

* 100 x (DeCART-Serpent) / DeCART)

Figure 3 shows a comparison of neutron pin power relative error distributions between Serpent 2 and DeCART2D calculations for four different burnup stages: 0, 10, 20, and 50 MWd/kg. The burnup steps of 0, 10, and 20 MWd/kg cover the Gd depletion period while50 MWd/kg burnup represents the expected maximum discharge burnup for the FA.

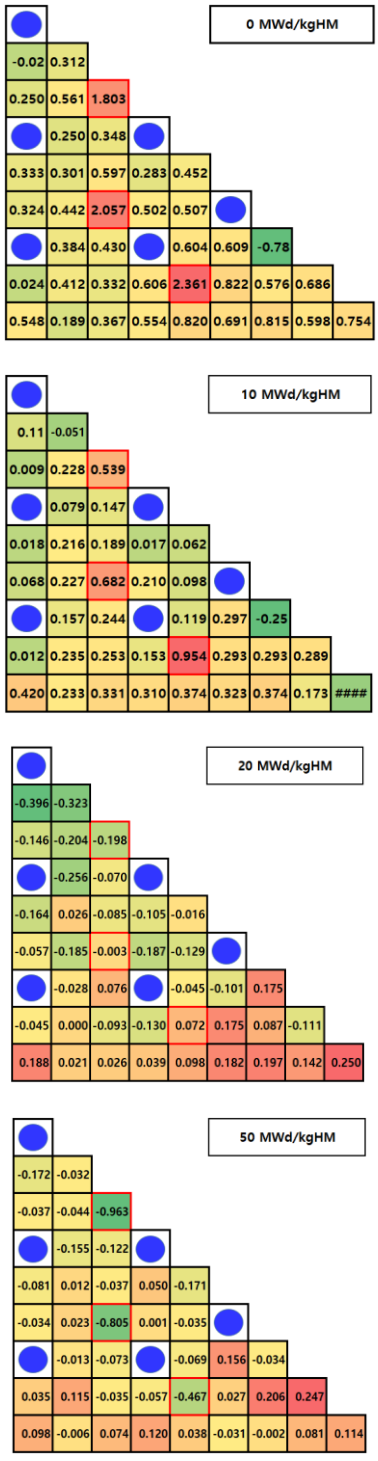

Fig. 3 Comparison of neutron pin power relative error distribution for four different burnup steps (0, 10, 20, 50 MWd/kg)

In the figure, the red border cells represent the positions of Gd fuel pins. Before Gd depletion, these pins show relatively larger difference between the two codes. However, after Gd depletion, the errors in Gd positions decrease, falling within 1% of each other. For the normal fuel pins, the agreement between Serpent 2

and DeCART2D is consistently good across all burnup steps with errors remaining below 1%.

Overall, the observed agreement in power distribution, coupled with the close match in the homogenized 2-group constants shown in Table III, provides strong evidence of the accuracy and reliability of the DeCART2D calculations. This level of agreement suggests that DeCART2D can be used for generating group constants in assembly-level calculations, which are crucial for subsequent core-level analyses.

Table IV : Summary of branch calculation

Parameter	**Variation**		Reference
Fuel Temperature (K)	**600**	**1200**	900
Moderator Temperature (K)	**500**	**650**	600

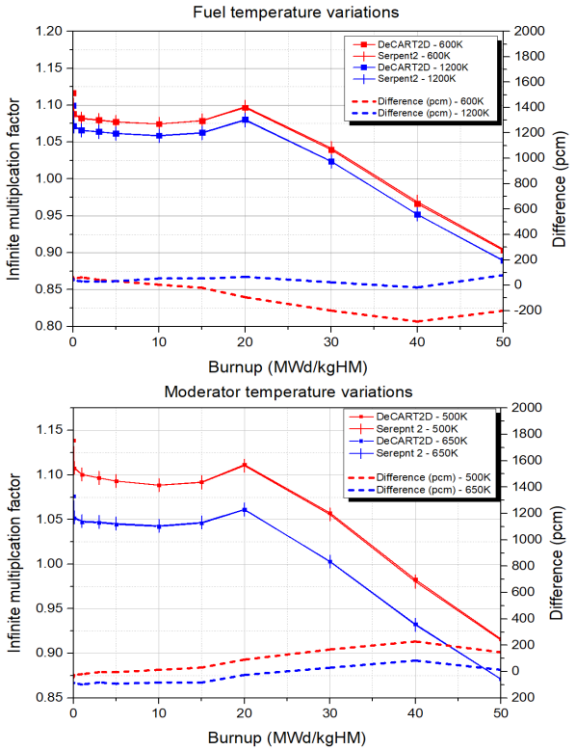

Fig. 4 Comparison of infinite multiplication factor evolutions for fuel and moderator temperature variations

Lastly, Table IV summarizes the branch calculation conditions, showing fuel temperature variations of 600K and 1200K (with a reference of 900K), and moderator temperature variations of 500K and 650K (with a reference of 600K). In Figure 4, the solid lines represent the comparison between the two codes (Serpent 2 and DeCART2D), while the dashed lines indicate the differences between them.

For fuel temperature variations, the results showed a maximum difference of -285 pcm between Serpent and DeCART2D at a burnup of 40 MWd/kg when the fuel temperature was 600K. At 1200K, the difference was smaller, at 66 pcm, observed at 20 MWd/kgHM. Regarding the moderator temperature variations, a difference of 228 pcm was noted at 40 MWd/kgHM burnup for 500K, while at 650K, the difference increased to -98 pcm at 1 MWd/kgHM burnup.

These results indicate that the branch calculations also showed reasonably good agreement between Serpent 2 and DeCART2D.

4. Conclusion and future work

In this study, a comprehensive comparison of neutronics parameters was conducted between Serpent 2 and DeCART2D codes to validate the reliability of group constants generated using DeCART2D. The results demonstrated good agreements between the two codes across multiple parameters, including k-values, pin power distributions, and group constants. This consistency provides the confidence in the reliability of DeCART2D for generating group constants in neutronics calculations for PWR applications, particularly for SBF SMR core designs.

Future work will focus on incorporating gamma smeared power distribution into the analysis. This enhancement will provide a more realistic representation of pin power distribution within the fuel assembly, accounting for gamma heating effects.

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REFERENCES

[1] Leppänen, Jaakko. "Serpent–a continuous-energy Monte Carlo reactor physics burnup calculation code." VTT Technical Research Centre of Finland 4.455 (2013): 2023-09.

[2] Kang, Han Ok, Byung Jin Lee, and Sang Gyu Lim. "Light water SMR development status in Korea." Nuclear Engineering and Design 419 (2024): 112966.

[3] J. Y. Cho et al., “DeCART2D v1.0 User’s Manual”, KAERI/TR-5116/2013