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Adaptation of Critical Buckling by Monte Carlo Method to DeCART2D Calculations for TCA Critical Facility

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1. Introduction

Recently, KAERI (Korea Atomic Energy Research Institute) developed its own two-step code coupling system using the DeCART2D lattice transport code [1] and MASTER nodal diffusion code [2] for a nuclear design and analysis. As part of the development, KAERI has prepared critical experiments for code licensing for the DeCART2D code system, concurrently. For verification and validation, the few group constants and pin-to-box factor by DeCART2D will be compared with the experimental results. Meanwhile, because the DeCART2D code treats only two-dimensional geometric information, a critical buckling and group-wise diffusion coefficients should be provided to consider the effect of axial leakage.

In the study, critical buckling will be generated through two approaches based on Monte Carlo (MC) calculations. The first way to generate critical buckling is by using the extrapolated length through a direct three-dimensional (3D) MC calculation. The alternative way is using the B_1 theory-augmented MC method [3]. To verify the critical buckling generated by the MC methods, the TCA (Tank-type Critical Assembly) benchmark problem was considered because it provides the measured values for the critical water level and extrapolation length [4].

2. Methods

2.1 Critical Buckling Generation by B_1 method

In common, the B_1 equations for a fine group (i.e., 47 and 190 group) can be expressed by

$$\begin{aligned} \Sigma_{t,g}\phi_g \pm iBJ_g &= \sum_{g'}(\Sigma^0_{gg'} + \chi_g \nu\Sigma_{f,g'})\phi_{g'} \\ \pm iB\phi_g + 3\alpha_g(B)\Sigma_{t,g}J_g &= 3\sum_{g'}\Sigma^1_{gg'}J_{g'} \end{aligned} \tag{1}$$

$$\alpha_g(B) = \begin{cases} \dfrac{1}{3}x^2\left(\dfrac{\arctan(x)}{x-\arctan(x)}\right) & \text{for } x^2 = \left(\dfrac{B}{\Sigma}\right)^2 > 0 \\ \dfrac{1}{3}x^2\left(\dfrac{\ln((1+x)/(1-x))}{\ln((1+x)/(1-x))-2x}\right) & \text{for } x^2 = -\left(\dfrac{B}{\Sigma}\right)^2 > 0 \end{cases} \tag{2}$$

where $\Sigma_{t,g}$ is the total macroscopic cross section and $\Sigma_{f,g}$ is the fission macroscopic cross section for the *g*-th energy group, respectively. Here, $\Sigma^n_{gg'}$ indicates a group-to-group scattering cross section for *n*-th order *Legendre* components. With the B_1 method, 0-th and 1-st order group-to-group scattering cross sections are used. The other notations are standard. In a conventional MC code, the fine group cross sections for solving B_1 equations are generated by the track length estimation or collision estimation method. The buckling (*B*), calculated by iterating it until *k* becomes 1, yields a critical buckling. Reference [3] covers this procedure in detail.

2.2 Direct Fitting Method by Axial Flux Distribution along the Core Height

In the experiment, the value of the axial buckling for a critical condition can be calculated using the extrapolated length from the activation measurements. In a finite cylinder reactor, normalized flux distributions for the vertical axis can be described well using a sinusoid with the extrapolated length. If a finite cylinder reactor has an extrapolated height *H'* and is centered about z=0, the flux distribution and geometric buckling can be written as

$$\phi(z) = \phi(0)\cdot\cos\left(\frac{\pi z}{H'}\right) \tag{3}$$

$$B_z^2 = \left(\frac{\pi}{H'}\right)^2 \tag{4}$$

$$H' = H + \lambda \tag{5}$$

where *H* is the height of the core in a finite cylinder reactor and λ is the extrapolated length or distance. In the same manner as the experiment, it is possible to obtain axial critical buckling from an axial flux distribution, ϕ_{MC}, which is calculated using the 3D MC calculation for the critical condition. The extrapolation length can be determined through a direct fitting method for a cosine function. It attempts to minimize the sum of the squares of the difference between ϕ_{MC} and the value (ϕ_{FIT}) from the fitted cosine function at the same height position. Equation 6 shows the definition of the root mean square (RMS) difference between ϕ_{MC} and ϕ_{FIT}.

$$R = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\phi^i_{MC} - \phi^i_{FIT}\right)^2} \tag{6}$$

where N and i indicate the total number of axial tallies and the index number, respectively.

3. Critical Buckling Generation for TCA Problem

3.1 TCA Benchmark

To examine the critical buckling by the above-mentioned two approaches based on the MC method, the TCA benchmark problems of the Japan Atomic Energy Research Institute (JAERI) are considered. Among the TCA benchmarks based on reference [4], two experimental cases are considered. In this case, the TCA facility has a single fuel assembly of 17x17 2.6 w/o enriched UO_2 fuel pins and is surrounded by light water in a 1.8-diameter core tank. The radius and pitch of the fuel pin are 0.625 and 1.956 cm, respectively. For convenience, we call the selected two benchmarks “problem I” and “problem II”. Figure 1 shows the configuration of the TCA core for each case.

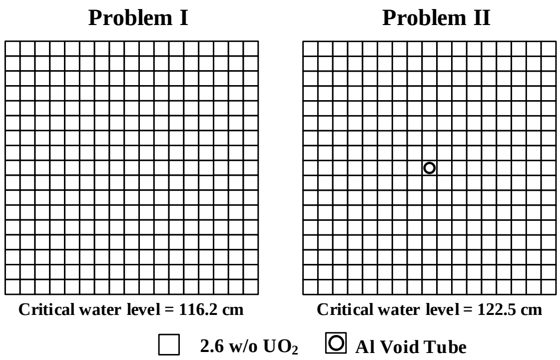

Fig. 1. Configuration of selected two TCA benchmarks

The only difference between two configurations is that the central fuel rod is replaced by an aluminum void tube. Table I shows the critical water level and measured extrapolation length for each problem.

Table I: Description of critical water level and extrapolation length for TCA Problem I and II

Case	Critical water level (cm)	Measured Extrapolation Length (cm)
Problem I	116.2	12.1±0.3
Problem II	122.5	12.3±0.3*

* Extrapolation length from problem II is obtained by inverse operation from the measured buckling

3.2 Critical Buckling for TCA Benchmark

Using the B_1 theory-augmented MC method and the direct fitting method, the axial critical buckling for two TCA problems are generated using the McCARD [5] code. All MC calculations with 100 active cycles and 100,000 histories per cycle are performed. For fission source convergence, 50 inactive cycles are used. The continuous energy cross section libraries are processed from ENDF/B-VII.1. The structure of fine group for the B_1 calculation adopts the 47 group structure of HELIOS [6]. Table II shows the critical buckling calculated by McCARD and the references. In the direct fitting method, the tally region is axially divided into one hundred cells. Through the direct fitting method, it is possible to express the axial flux distributions for each problem as below

$$\phi_{FIT}^{I}(z) \approx 1.77\cos(\frac{\pi}{129.6}z - 1.38) \quad (7)$$

$$\phi_{FIT}^{II}(z) \approx 1.71\cos(\frac{\pi}{133.8}z - 1.39) \quad (8)$$

where $\phi_{FIT}^{I}(z)$ and $\phi_{FIT}^{II}(z)$ are the direct fitted axial flux distribution functions for problems I and II, and z=0 at the bottom of the active core. In either case, the RMS differences (R) are less than 0.9%.

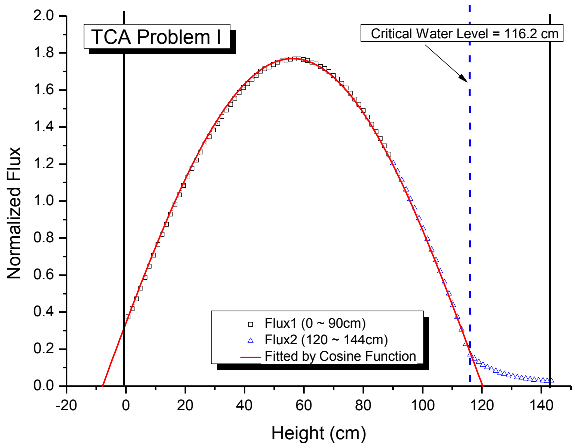

Fig. 2. Direct axial flux distribution fitting for problem I

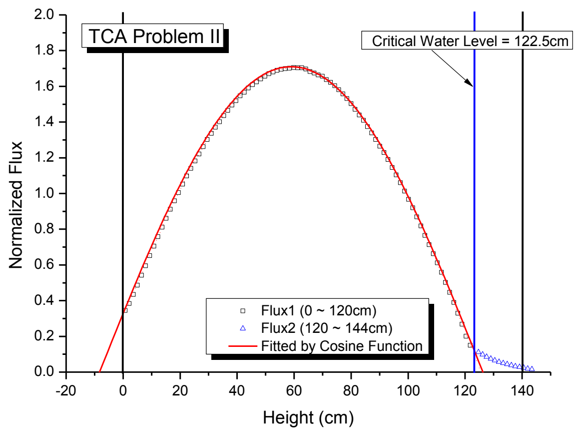

Fig. 3. Direct axial flux distribution fitting for problem II

As shown in Figs. 2 and 3, the fitted cosine functions (*orange line*) and the flux distributions (*black dots*) by the 3D MC calculations show excellent agreement. In problem I, the relative differences of the B_1 theory-augmented MC method and the direct fitting method are -3.3% and -1.8%, respectively. In problem II, the relative difference are -0.2% and 1.5%, respectively. Considering that statistical uncertainties of the critical buckling by McCARD is less than 0.11%, there is no significant difference between the MC-generated buckling and reference.

Table II: Vertical critical buckling by the two MC methods for TCA Problems I and II

Case	REF[4]	McCARD*	
		B_1**	FIT***
Problem I	5.986×10^{-4} $\pm2.8\times10^{-6}$	5.789×10^{-4}	5.876×10^{-4}
Problem II	5.429×10^{-4} $\pm2.4\times10^{-6}$	5.437×10^{-4}	5.513×10^{-4}

* The statistical uncertainty by McCARD is less than 2.0×10^{-5}.
** B_1 theory-augmented MC method
*** Direct fitting method by 3D MC calculations

3.3 DeCART2D Calculation with Critical Buckling

To examine the MC-generated axial critical buckling, DeCART2D calculations are performed for each problem. The DeCARTD2D calculations are conducted using the ENDF/B-VII.1 based 47-group cross section library [7], the direct iteration method with a resonance integral table, and the default ray tacking option. For consideration of its leakage effect, the group-wise diffusion coefficients are generated through the DeCART2D calculations.

Table III: k_{eff} by DeCART2D calculations with critical buckling for TCA problems I and II

Case	k_{eff} by DeCART2D		
	REF*	B_1**	FIT***
Problem I	0.99905	0.99967	0.99940
Problem II	1.00094	1.00092	1.00068

* By critical buckling from reference 4
** B_1 theory-augmented MC method
*** Direct fitting method by a 3D MC calculation

Table III shows the k_{eff} of the TCA benchmark problem by DeCART2D using the critical buckling as shown in Table II. The k_{eff} values obtained with the McCARD generated critical buckling are much closer to the criticality (1.0) than those obtained with the reference. The maximum error of k_{eff} obtained with the McCARD one is less than 100 pcm. From all of the results, it was verified that the two MC method works reasonably well.

	1.515 1.497 -1.2%	1.359 1.337 -1.7%	1.277 1.255 -1.8%	1.193 1.174 -1.6%	1.096 1.084 -1.1%	0.997 0.994 -0.3%	0.942 0.949 0.8%	1.122 1.096 -2.4%
	1.418 1.400 -1.3%	1.335 1.313 -1.7%	1.265 1.242 -1.9%	1.183 1.164 -1.6%	1.087 1.075 -1.1%	0.987 0.986 -0.1%	0.936 0.941 0.5%	1.112 1.087 -2.3%
		1.290 1.268 -1.8%	1.230 1.208 -1.8%	1.153 1.135 -1.6%	1.067 1.049 -1.8%	0.964 0.962 -0.2%	0.912 0.918 0.6%	1.084 1.060 -2.2%
			1.176 1.157 -1.7%	1.103 1.087 -1.5%	1.014 1.005 -0.8%	0.921 0.922 0.1%	0.873 0.880 0.7%	1.038 1.016 -2.2%
				1.032 1.023 -0.9%	0.950 0.946 -0.5%	0.864 0.868 0.4%	0.820 0.828 1.0%	0.974 0.956 -1.9%
					0.873 0.875 0.2%	0.794 0.803 1.0%	0.753 0.766 1.6%	0.895 0.884 -1.3%
						0.723 0.736 1.8%	0.684 0.701 2.4%	0.810 0.805 -0.6%
	McCARD DeCART2D Diff(%)						0.644 0.663 3.0%	0.744 0.747 0.4%
								0.790 0.787 -0.4%

Fig. 4. Comparison of pin power distribution by DeCART2D with the critical bucking from the reference 4 (REF) for problem II

Figure 4 shows the accuracy of the DeCART2D with the critical buckling from reference [4] (REF) in terms of the pin power estimations in problem II. The RMS and maximum relative difference for all pin powers are shown to be 1.5% and 3.0%, respectively. Table IV compares the RMS difference with varying the critical buckling for problems I and II.

Table IV: RMS difference of pin power distribution between McCARD and DeCART2D

Case	RMS difference (%)		
	REF*	B_1**	FIT***
Problem I	1.9	1.9	1.9
Problem II	1.5	1.5	1.5

* By critical buckling from reference 4
** B_1 theory-augmented MC method
*** Direct fitting method by a 3D MC calculation

3. Conclusions

In this study, the B_1 theory-augmented MC method and the direct fitting method using a 3D MC calculation to generate an axial critical buckling were introduced and examined by the TCA critical experiment benchmark. From the results of two TCA benchmark problems, it should be noted that DeCART2D with the critical buckling by the two MC methods predicts the criticality very well. Because the MC method has the merit of using a continuous energy nuclear cross section and handling detailed geometric data, the two methods will be utilized as an effective way to provide the axial critical buckling for a new-type reactor that lacks experimental measurements.

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