Feasibility of 2-D GPS Functions in 3-D Benchmark Problems

Jaeha Kim, Hwanyeal Yu, and Yonghee Kim Korea Advanced Institute of Science and Technology (KAIST) 291 Daehak-ro, Yuseong-gu, Daejeon, Korea, 34141 *Corresponding author: yongheekim@kaist.ac.kr

1. Introduction

Basically, a core analysis based on the neutron diffusion theory is based on the group constants generated by assembly-wise lattice calculations using the neutron transport theory, and such core analysis procedure is called the conventional two-step procedure. However, since the group constants, cross sections (XS) and discontinuity factors (DF), are generated using the unrealistic reflective boundary condition, there is an inevitable error in the conventional two-step procedure. In the case of the pin-wise group constants, the error is more significant and this is why the pin-by-pin diffusion analysis has not been in the mainstream.

Recently, a new leakage correction method, called GET plus SPH (GPS) method was proposed to reduce the error of conventional two-step procedure in pin level. By combining the generalized equivalence theory (GET) [1] and the super-homogenization method (SPH) [2], the modified SPH concept was introduced to correct the pinwise cross sections obtained by assembly-wise lattice calculations. The feasibility of the GPS method in 2-D geometries has been demonstrated in the previous studies [3,4].

In this work, the feasibility of the GPS functions generated by the 2-D color-set calculations is analyzed by adapting them to several 3-D benchmark problems.

2. GPS Method

In the GPS method, the pin-wise and XS-wise SPH factor concept is introduced to correct the pin-wise XSs generated by a single-assembly lattice transport calculation based on the standard GET. The pin-wise and XS-wise SPH factors of the GPS method are evaluated in various color-set models which consist of several types of fuel assembly located next to each other. In each color-set model, the pin-wise SPH factors for each assembly type that satisfy Eq. (1) are obtained by the color-set SPH iteration of repeated pin-wise diffusion calculations and XS updates as shown in Fig. 1.

 $\tau_{g,x}^{color-set} = SPH_{g,x} \sum_{g,x}^{SA} \phi_{g,dif}^{color-set}$ (1)

where

g = Group index, x = Reaction type index, $\tau_{g,x}^{color-set} = Reference pin-wise reaction rate by tranport calc.,$ $\phi_{g,df}^{color-set} = Pin-wise flux by nodal diffusion calc.,$ $\Sigma_{g,x}^{SA} = Pin-wise XS by single-assembly tranport calc.,$ $SPH_{g,x} = XS-wise SPH factor.$



Fig. 1. GPS function fitting data generation (color set)

In the GPS method, the SPH factors are parameterized as a function of pin-wise two-group current-to-flux ratio (CFR) which is defined by Eq. (2) in 2-D geometry and Eq. (3) in 3-D geometry. In this work, the node-wise flux and surface-wise out-going net currents are appropriately weighted by area and length in a 2-D case, or volume and area in a 3-D case, so that the two definitions for each dimension are equivalent and compatible.

$$CFR_{g}^{2D} = \frac{\sum_{s} J_{g}^{s} \cdot l^{s}}{\phi_{g} \cdot A} = \frac{\sum_{s} J_{g}^{s} \cdot l^{s}}{\phi_{g} \cdot A} \times \frac{h}{h} = \frac{\sum_{radials} J_{g}^{s} \cdot A^{s}}{\phi_{g} \cdot V}$$
(2)
$$CFR_{g}^{3D} = CFR_{g}^{2D} + \frac{\sum_{axials} J_{g}^{s} \cdot A^{s}}{\phi_{g} \cdot V}$$
(3)

where

l =Node radial pitch length,

A = 2-D node area,

h = Node axial height,

V = 3-D node volume.

In this work, the changes of the pin-wise SPH factors, Eq. (4), are functionalized by the changes of the two-group CFR, Eq. (5).

$$\Delta SPH_{g,x} = SPH_{g,x}^{color-set} - SPH_{g,x}^{SA}$$
(4)

$$\Delta CFR_g = CFR_g^{color-set} - CFR_g^{SA} \tag{5}$$

As specified in Eq. (4) and (5), the changes mean the differences of those values in each reference color-set calculation and the single-assembly lattice calculation. Naturally, the CFR values in the lattice calculations are zero due to the full reflective boundary condition. Meanwhile, the SPH factors in the lattice calculation are considered to be 1.0, since the pin-wise DFs generated by the lattice calculation. The pin-wise DFs are to preserve

the heterogeneous quantities in a lattice geometry, and it means one do not need any further XS correction using non-unity SPH factors.

The detailed two-group GPS functions are as in Eq. (6) and (7). The coefficients for both group delta CFR values and a constant term are obtained by the color-set fitting data sets.

$$\Delta SPH_{F,x} = a_{1,F,x} \Delta CFR_{F,x} + a_{2,F,x} \Delta CFR_{F,x} + a_{3,F,x}$$
(6)

$$\Delta SPH_{T,x} = a_{1,T,x} \Delta CFR_{F,x} + a_{2,T,x} \Delta CFR_{F,x} + a_{3,T,x}$$
(7)

With the pre-defined pin-wise and XS-wise GPS functions for each assembly type, the XSs are updated once as in Eq. (8) using the pin-wise CFR information evaluated from an initial steady-state calculation. The overall flowchart of the GPS method is briefly described in Fig. 2.

$$\Sigma_{g,x}^{corrected} = (1 + \Delta SPH_{g,x}) \cdot \Sigma_{g,x}^{SA}$$
(8)



Fig. 2. Flowchart of the GPS method

Previously, the GPS functions generated by 2-D colorset calculations have been used only in 2-D benchmark problems. In this work, the feasibility of the 2-D GPS functions are analyzed by adapting them in several 3-D benchmark problems.

3. Numerical Results

A 2-D method of characteristics (MOC) based lattice code, DeCART2D [5] was used for the lattice calculations and color-set calculations for GPS functionalization. The 3-D pin-by-pin diffusion analyses were performed by an in-house NEM-based pin-wise nodal code with the hybrid CMFD (HCMFD) algorithm [6]. The reference core calculations were performed by a continuous energy Monte Carlo (MC) code, SERPENT [7] with the ENDF/B-VII.1 library.

It should be mentioned that the computer codes for the reference solution and the GPS functionalization, SERPENT and DeCART2D, are different. Thus, the error between the corrected diffusion solution and the reference MC solution probably contains the error between those two codes. In the near future, the GPS functions by DeCART2D will be replaced by those by SERPENT for consistency.

The 2-D benchmark problems which are treated in the previous works as described in Fig. 3 to 6 were extended to 3-D, Problem 1 to 3, with the axial reflector layers at the top and bottom of the active core. The detailed 3-D quarter core geometry is described in Table I. The Axial DFs are only considered on the interface between the axial reflector layers and fuel assemblies. In the diffusion calculations, the axial mesh size was fixed to 20cm.

Table I: 3-D quarter core geometry

	1 2	
Radial configuration	No. of assemblies	13
	No. of	10
	baffle/reflector nodes	12
Axial configuration	Top reflector	20cm×1
	Active core	20cm×10
	Bottom reflector	20cm×1
Assor	21.42cm×21.42cm	
Assel	(17 by 17 pins)	



Fig. 3. UOX fuel assembly geometry (KAIST-1A)

	Reflective BC						
	UOX-2 BA16	UOX-2	UOX-2 BA16	UOX-1			
BC	UOX-2	UOX-1	UOX-2	UOX-1		Ve	
lective	UOX-2 BA16	UOX-2	UOX-1			icuum E	
Ref	UOX-1	UOX-1				ŝ	
	Vacuum BC						

Fig. 4. Fuel loading pattern 1 (Problem 1)



Fig. 5. Fuel loading pattern 2 (Problem 2)



Fig. 6. Fuel loading pattern 3 (Problem 3)

First, the k_{eff} values without and with the GPS correction were compared with the reference values in each problem, and the results are presented in Table III. The results without the GPS correction is the initial steady-state results, the standard two-step calculation. The changes in k_{eff} error are quite comparable to those in 2-D benchmarks of previous study [3], which uses the same GPS functions. It expected that the 2-D GPS functions are working quite well in 3-D problem.

Toblo.	III.	1 and	00000	aom	noricon
rable	ш.	K _{eff} and	enor	COIII	parison

Туре	k _{eff}	error (pcm)			
Problem 1					
Ref. (SERPENT)	1.099221	-			
w/o GPS	1.100301	+107.99			
with GPS	1.099498	+27.68			
Problem 2					
Ref. (SERPENT)	1.041678	-			
w/o GPS	1.042670	+99.21			
with GPS	1.042155	+47.79			
Problem 3					
Ref. (SERPENT)	1.042212	-			
w/o GPS	1.042987	+77.55			
with GPS	1.042655	+44.34			

To analyze the results in more detail, the pin power errors were compared in layer-by-layer sense. Prior to introducing the 3-D results, the changes in the RMS and maximum pin power error in 2-D benchmarks are presented in Table IV. In a similar way, the 3-D results are presented in Table V to VII in layer-by-layer sense.

Basically, the overall pin power error is larger in 3-D problems since the pin power peaking factor is usually larger in 3-D problems than in 2-D problems. The pin power error can easily be amplified in pins with very small level of power, and it is quite clearly observed in view of the maximum pin power error of each layer. The maximum errors are even more than 30% at the top layers in Problem 2 and 3, where the top layers contain the fuel pin of the weakest power. Moreover, it is noted that the XSs and DFs of the axial reflector layers are

generated using a simplified 2-D geometry, and it can cause additional error.

It is noteworthy that the pin power RMS errors especially at the central layers are quite improved from ~1.5% to ~1.1% by the GPS corrections, where it is comparable to those of 2-D problems. It indicates the 2-D GPS functions can correct the XSs quite well since the axial neutron leakages are sufficiently small at the central layers. Meanwhile, the RMS errors at the top and bottom boundary layers even increase after the GPS correction in Problem 1.

Table IV: Pin power error (2-D)

Loading pattern #	Pin power		Pin power	
	RMS error (%)		maximum error (%)	
	w/o GPS	with GPS	w/o GPS	with GPS
1	0.82	0.21	2.95	1.64
2	0.77	0.26	2.75	1.30
3	0.82	0.28	2.76	1.20

Table V: Layer-wise pin power error (Problem 1)

	Pin power		Pin power	
Layer #	RMS error (%)		maximum error (%)	
	w/o GPS	with GPS	w/o GPS	with GPS
10 (Top)	2.41	2.62	22.74	14.31
9	1.91	1.49	6.85	7.82
8	1.72	1.25	6.53	7.40
7	1.63	1.17	6.40	7.21
6	1.56	1.09	6.26	6.91
5	1.56	1.08	6.36	6.92
4	1.54	1.10	6.28	6.69
3	1.64	1.19	6.29	7.13
2	1.74	1.30	6.72	7.55
1 (Bottom)	1.87	2.04	11.71	9.49
Total	1.78	1.51	22.74	14.31

Table VI: Layer-wise pin power error (Problem 2)

	Pin power		Pin power	
Layer #	RMS error (%)		maximum error (%)	
	w/o GPS	with GPS	w/o GPS	with GPS
10 (Top)	3.06	2.60	38.11	24.67
9	1.76	1.28	7.05	8.06
8	1.50	1.06	6.21	7.03
7	1.48	1.07	6.49	7.25
6	1.47	1.08	5.95	6.74
5	1.47	1.09	5.98	6.70
4	1.51	1.06	6.05	6.71
3	1.56	1.07	6.11	6.88
2	1.70	1.19	6.70	7.55
1 (Bottom)	2.10	1.99	20.84	12.95
Total	1.82	1.44	38.11	24.67

	Pin power		Pin power	
Layer #	RMS error (%)		maximum error (%)	
	w/o GPS	with GPS	w/o GPS	with GPS
10 (Top)	3.63	3.01	37.13	23.36
9	2.29	1.51	7.59	8.29
8	2.02	1.20	6.42	7.33
7	1.82	1.07	6.15	6.52
6	1.78	1.07	6.12	6.99
5	1.77	1.07	5.93	6.84
4	1.83	1.10	5.62	6.64
3	1.87	1.13	6.94	7.99
2	2.01	1.22	6.61	7.63
1 (Bottom)	2.53	2.10	21.29	12.20
Total	2.22	1.57	37.13	23.36

Table VII: Layer-wise pin power error (Problem 3)

The radial pin power error distributions in Problem 2 at layer 5 without and with the GPS correction are plotted together in Fig. 7. It clearly shows the overall pin power error is improved by the GPS correction. Meanwhile, the red dots are the fuel pins including the burnable absorber, and it was figured out that such larger error especially in the burnable absorber pins is caused by the error between DeCART2D and SERPENT, where the absorption rate estimations of each code are quite different.



Fig. 7. Radial pin power error at layer 5 (Problem 2)

4. Conclusions

It was demonstrated that the GPS functions generated by 2-D color-set calculations can also be utilized in 3-D geometries consist of the same assembly types without any critical problem. Currently, the effectiveness of the 2-D GPS functions in 3-D problems is limitedly figured out at the central layers where the axial neutron leakage is relatively small. The results will be reproduced soon with the consistency between the color-set calculation and reference calculation using SERPENT. As a further work, the 3-D GPS functions generated by 3-D color-set models will be considered.

ACKNOWLEDGMENTS

This work was supported by the National Research Foundation of Korea (NRF) Grant funded by the Korean Government (MSIP) (NRF-2016R1A5A1013919).

REFERENCES

[1] K. S. Smith, "Assembly Homogenization Techniques for Light Water Reactor Analysis," *Progress in Nuclear Energy*, 17, 303, 1986.

[2] A. Hebert, "A Consistent Technique for the Pin-by-Pin Homogenization of a Pressurized Water Reactor Assembly", *Nucl. Sci. Eng.*, 113, 227, 1993.

[3] H. Yu, W. Kim, and Y. Kim, "A Leakage Correction with SPH Factors for Two-group Constants in GET-based Pin-by-Pin Reactor Analyses", *Annals of Nuclear Energy*, Vol. 129, p. 30-50, July, 2019.

[4] HwanYeal Yu, Jaeha Kim, and Yonghee Kim, "Pinwise Diffusion Solution of Partially MOX-Loaded PWRs with the GPS (GET PLUS SPH) Method," *Nuclear Science and Engineering*, Published online, 10 June, 2019.

[5] "DeCART 2D v1.0 User's Manual," KAERI/TR-5116/2013, Korea Atomic Energy Research Institute, 2013.

[6] J. Leppanen, "PSG2 / Serpent - a Continuous-energy Monte Carlo Reactor Physics Burnup Calculation Code," VTT Technical Research Centre of Finland, 13 June, 2012.

[7] Jaeha Kim, and Yonghee Kim, "Development of 3-D HCMFD algorithm for efficient pin-by-pin reactor analysis," *Annals of Nuclear Energy*, vol. 127, 87-98, 2018.

[8] N. Z. Cho, "Benchmark Problem 1A: MOX Fuel-Loaded Small PWR Core (MOX Fuel with Zoning)", KAIST/NuratT, 23 June, 2000.