Estimation of the Correction Effect of SPH method in Diffusion and SP_3 theory

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1. Introduction

In recent years, owing to the growth of the computing power, various researches concerning the direct whole core calculation (DWCC) codes have been performed to obtain the accurate core calculation results by solving neutron transport equation. However, the DWCC codes are still yet impractical for reactor designs and analyses which require thousands of core calculations. It is the prime reason that the conventional two-step method which requires low computing cost remains as the major tool in the nuclear industries.

In order to maintain the advantage of the two-step method while exploiting the increased computing power, pin-wise two-step core analysis method has been widely developed. In this regard, the second class of the two-step method is developed by combining the nTRACER DWCC code [1] and SPHINCS [2], pin-wise simplified P_3 (SP_3) code, which employs the 2D/1D finite difference method (FDM) solver coupled with the assembly-wise coarse mesh finite difference kernel to reduce the computing cost. Not only the SP_3 but also the diffusion theory is widely used for high performance pin-by-pin core calculations [3] and the SPHINCS code can also perform the diffusion-based pin-wise core analysis as an additional option.

Although nTRACER was originally developed for the DWCC employing the method of characteristics (MOC), it can be used as a lattice transport code which can generate not only the pin-homogenized group constants (PHGCs) but also the reference solutions. The errors resulting from the generation of PHGCs are corrected by the super homogenization (SPH) [4] method.

The SPH method has been widely used in pin-by-pin calculations such as SCOPE2 [5] and DYN3D [6] due to its simplicity. However, it should be aware that various errors from different origins, including the spatial homogenization, group condensation, spatial discretization, and low order transport approximation are simultaneously corrected [7]. It is why the use of more elaborated solution method does not guarantee the improvement of accuracy. For example, the SP_3 solver with pin-sized FDM can yield larger error than the diffusion, depending on the problem, since the reduction of transport approximation error can weaken the error cancellation so that the other errors can be emerged.

In this regard, this study aims to estimate the correction effect of SPH method for both diffusion and SP_3 using the deviation of group-wise SPH factors as a measure.

2. Correction by the SPH Method

2.1. Four errors of the pin-wise two-step method

PHGCs are obtained by the heterogeneous lattice transport solver, while the two-step calculations are performed for homogenized domain by lower order solvers. The inconsistency leads to the following four errors: the lower order transport approximation error due to the use of diffusion or SP_3 theory, the spatial discretization error related with the FDM mesh size, the group condensation error determined by the number of collapsed energy group, and the spatial homogenization error due to the loss of heterogeneous pin-cell geometry.

Among the four errors, the degree of the transport and the discretization effects are estimated for the diffusion and SP_3 FDM solvers with different sub pin-cell mesh refinement options, using the deviation of SPH factors as the indicator.

2.2. Deviation of SPH factors

The lattice transport calculations are performed for the explicitly modeled assembly. Each pin-cell is divided into tens of flat source regions (FSRs) and the resulting FSR-wise fluxes are used to generate PHGCs. With given PHGCs and fluxes, the group-wise SPH factors for each pin defined as the ratio of the heterogeneous flux to the homogeneous flux as Eq. (1) are obtained in an iterative procedure while preserving the group-wise total reaction rates at each pin.

$$\bar{\Sigma}_{m,g}\bar{\phi}_{m,g} \neq \bar{\Sigma}_{m,g}\bar{\phi}^{*}_{m,g} \rightarrow \varsigma_{m,g} = \frac{\bar{\phi}^{*}_{m,g}}{\bar{\phi}_{m,g}},$$
$$\tilde{\Sigma}_{m,g} \equiv \varsigma_{m,g}\bar{\Sigma}_{m,g} \rightarrow \tilde{\Sigma}_{m,g}\bar{\phi}_{m,g} = \bar{\Sigma}_{m,g}\bar{\phi}^{*}_{m,g} \quad (1)$$
$$\text{where } \bar{\phi}^{*}_{m,g} = \frac{\sum_{k\in m} V_k \phi^{het}_{k,g}}{\sum_{k\in m} V_k}.$$

In Eq. (1), ϕ^{het}_{k} and $\bar{\phi}^{*}_{m}$ are the heterogeneous neutron flux for each FSR k and their average over homogenized region, i.e., pin, m. $\bar{\phi}_{m}$ is homogeneous counterpart of

$\bar{\phi}_m^*$, $\bar{\Sigma}_m$ and ς_m denote PHGC and SPH factor of region *m* where *g* stands for the group index.

For each type of fuel assemblies, a single assembly (SA) calculation is performed in order to generate PHGCs and SPH factors. For the reflector regions, fuel-reflector configurations in Fig. 1 are used and the effect of the adjacent fuel assembly in the generation of PHGCs and SPH factors turned out to be negligible [2].

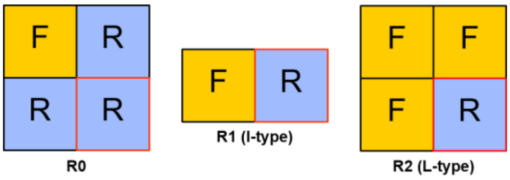

Fig. 1. Fuel-reflector configurations for the reflector PHGCs and SPH factors

The deviation of SPH factors are estimated as Eq. (2) where *i*, *g*, *N* stand for pin index, group index, and the total number of pins used in the SPH iteration, respectively. By the definition of SPH factors in Eq. (1), the deviation of SPH factors from unity can be used as a measure for the correction effect.

$$\sqrt{\frac{\sum_{i=1}^{N}\left(\frac{\bar{\phi}_{i,g}^{*}-\bar{\phi}_{i,g}}{\bar{\phi}_{i,g}}\right)^{2}}{N}} \qquad (2)$$

3. Numerical Results

3.1. Problem specifications

Three configurations in Fig. 2, namely Unrodded and Rodded-A and B, are loaded with the C5G7 [8] UO_2 and MOX assemblies.

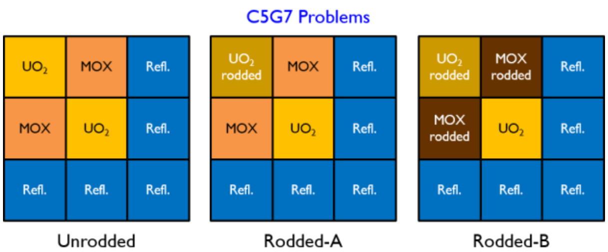

Fig. 2. Three types of modeled problems

As shown in Table I, for the heterogeneous solution, sub-pin level is explicitly modeled, while coarse and fine ray conditions are employed for the homogeneous solutions.

Table I: Calculation conditions for nTRACER

Heterogeneous	Explicitly modeled sub pin-cell geometry
	Ray spacing: 0.01cm No. of azimuthal angles: 32 No. of polar angles: 4
Homogeneous	Coarse ray conditions
	Ray spacing: 0.05cm No. of azimuthal angles: 8 No. of polar angles: 4
	Fine ray conditions
	Ray spacing: 0.01cm No. of azimuthal angles: 32 No. of polar angles: 4

The homogeneous solutions with fine ray conditions are set as the reference solution for the assessment of discretization and transport effect. In other words, with same PHGCs, the discretization effect is to be reduced as the fine-mesh structure is employed and only the transport effect of diffusion and SP_3 is compared with MOC. At last, the correction effect is estimated based on the deviation of SPH factors.

Table II: Procedures for the reduction of error causes

Error causes	Procedures
Spatial homogenization	Same PHGCs
Group condensation	
Spatial discretization	Fine-mesh structures
Transport method	MOC vs. Diffusion or SP_3

3.2. Need for equivalence factors (EFs)

The reference heterogeneous solutions can't be reproduced with PHGCs generated from SA calculations even though the transport solver with fine-mesh structures is used as shown in Table III. This is due to the fact that PHGCs are generated merely conserving the reaction rate at each pin and the leakage between the pin cells is not considered.

Table III: Discrepancy of results obtained with PHGCs compared to the heterogeneous solutions

ID	nTRACER Calculations				
	Hetero.	Homo. Coarse ray		Homo. Fine ray	
	k-eff.	k-eff.	$\Delta\rho$ (pcm)	k-eff.	$\Delta\rho$ (pcm)
Unrod.	1.18641	1.18405	-168.0	1.18742	71.7
Rod.-A	1.04904	1.04437	-426.3	1.04686	-198.5
Rod.-B	0.96359	0.95762	-647.0	0.95993	-395.7

The transport error can be estimated when the PHGCs are directly used with fine-mesh discretization. As shown in Table IV that 8x8 sub-meshes are employed for each pin, SP_3 shows much better results than diffusion especially for heavily rodded cases but the discrepancy of reactivity and pin power distribution is not negligible. Therefore, the need for EFs and better accuracy of SP_3 than diffusion is clearly shown.

Table IV: Comparison of the transport effect using same PHGCs with fine-mesh discretization respectively

Description	nT.	SPHINCS-Diffusion			
	k-eff.	k-eff.	$\Delta\rho$ (pcm)	ΔP (Max.)	ΔP (RMS)
Unrodded	1.18742	1.18562	-128.0	2.3	0.7
Rodded-A	1.04686	1.03756	-856.4	6.4	1.8
Rodded-B	0.95993	0.94752	-1364.7	7.9	2.4
Description	**nT.**	**SPHINCS-SP3**			
	k-eff.	k-eff.	$\Delta\rho$ (pcm)	ΔP (Max.)	ΔP (RMS)
Unrodded	1.18742	1.18699	-30.9	0.5	0.1
Rodded-A	1.04686	1.04470	-197.5	2.0	0.9
Rodded-B	0.95993	0.95688	-331.8	3.0	1.5

3.3. Comparison for the reduction of discretization error between diffusion and SP_3

Table V and Table VI present the reduction of discretization error solely by mesh refinement which are compared with the results obtained from nTRACER fine ray conditions and same PHGCs.

Unless sub-meshes are used, the diffusion shows better accuracy in aspects of reactivity and pin power compared to the SP_3. But when the sub-meshes are refined, the discretization error becomes reduced and only the transport error is shown. In that case, SP_3 shows much better accuracy than the diffusion especially for the case with steep flux gradient. To elaborate on this, the root-mean-square (RMS) error of pin power distribution of SP_3 is much smaller than that of diffusion in MOX assembly rather than in UO_2 assembly. The discrepancy between diffusion and SP_3 becomes even larger in case of the reflector (R0, R1).

Accordingly, the discretization error is reduced with sub-mesh refinement and it is clear that SP_3 shows better accuracy than diffusion in aspect of transport effect.

Table V: Comparison for the reduction of discretization error between diffusion and SP_3 for fuel assemblies

ID	SPHINCS discretization		$\Delta\rho$ (pcm)	ΔP (Max.)	ΔP (RMS)
UO_2	1x1	D	-91.9	0.39	0.22
		SP_3	-138.6	-0.51	0.27
	8x8	D	54.8	1.18	0.42
		SP_3	22.6	0.95	0.34
	32x32	D	57.5	1.19	0.42
		SP_3	26.4	0.96	0.35
MOX	1x1	D	-151.8	-1.97	0.80
		SP_3	-131.2	-2.55	1.10
	8x8	D	-62.4	1.48	0.74
		SP_3	-46.5	0.77	0.34
	32x32	D	-61.0	1.52	0.76
		SP_3	-44.6	0.80	0.36

Table VI: Comparison for the reduction of discretization error between diffusion and SP_3 for reflector assemblies

ID	SPHINCS discretization		$\Delta\rho$ (pcm)	ΔP (Max.)	ΔP (RMS)
R0	1x1	D	-967.6	2.21	0.97
		SP_3	-347.8	-4.31	1.77
	8x8	D	-591.1	4.91	1.54
		SP_3	44.8	1.71	0.66
	32x32	D	-584.4	5.00	1.57
		SP_3	53.4	1.68	0.68
R1	1x1	D	-440.2	-1.39	0.80
		SP_3	-235.3	-3.68	1.27
	8x8	D	-190.9	3.70	1.09
		SP_3	30.1	1.29	0.54
	32x32	D	-186.4	3.78	1.10
		SP_3	36.1	1.29	0.55

3.4. Deviation of SPH factors

Since SP_3 shows better accuracy than diffusion when the discretization error is reduced, the deviation of SPH factors is estimated as the sub-meshes are refined. The deviation of SPH factors from unity can be used as a measure so that the correction effect of those for diffusion and SP_3 can be compared.

Fig. 3 shows the distribution of SPH factors for Group 7 in UO_2 and MOX assembly. For both diffusion and SP_3, the deviation of SPH factors is decreased as the sub-meshes are refined. And for fine-mesh refinement, the deviation of SPH factors in SP_3 is smaller than that in diffusion.

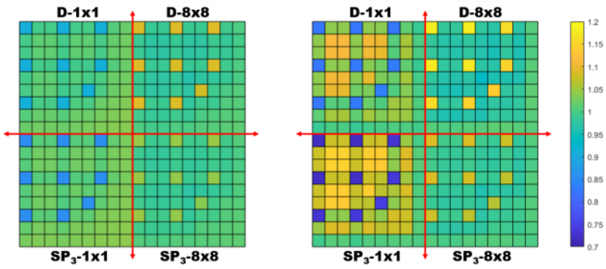

Fig. 3. Distribution of SPH factors (Group 7) for UO_2 (left) and MOX (right) assembly varying mesh refinement

Fig. 4 and Fig. 5 shows the group-wise deviation of SPH factors with 1x1 sub-mesh and 8x8 sub-meshes for fuel assemblies. Note that the broad and narrow bars are the results of diffusion and SP_3 respectively. As shown in Fig 4, the deviation of SPH factors in SP_3 is larger than that in diffusion especially in thermal energy group range. But it becomes much smaller in Fig 5 where 8x8 sub-meshes are employed. Accordingly, for the case that discretization error is reduced, SPH method only corrects for transport effect, and the degree of correction effect for the SP_3 is smaller than the diffusion.

This is also clearly shown for reflector assemblies in Fig. 6. There is no significant difference among mesh discretization but the correction effect of SPH method between the diffusion and the SP_3 shows remarkable difference.

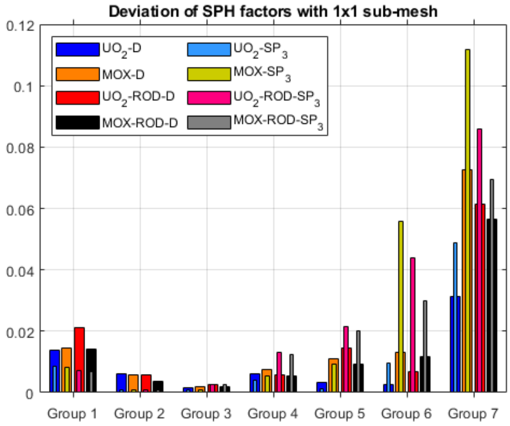

Fig. 4. Deviation of SPH factors with 1x1 sub-mesh for fuel assemblies

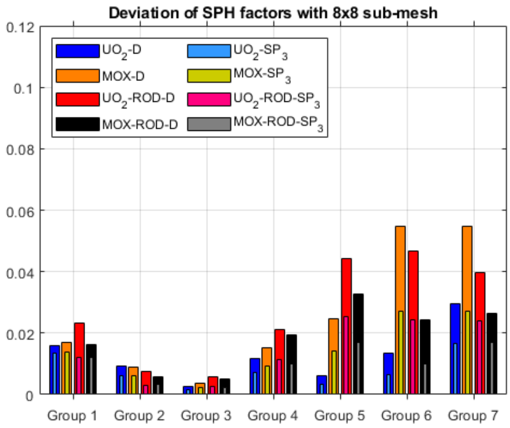

Fig. 5. Deviation of SPH factors with 8x8 sub-meshes for fuel assemblies

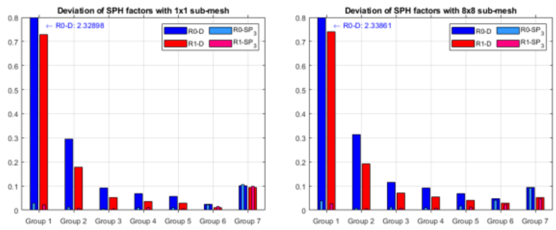

Fig. 6. Deviation of SPH factors with 1x1 sub-mesh (left) and 8x8 sub-meshes (right) for reflector assemblies

3.5. Effect of discretization in the generation of SPH factors on core analysis

The deviation of SPH factors is highly dependent on mesh refinement and the effect of discretization in the generation of SPH factors affects core analysis as well since the SPH factors obtained by Eq. (1) in fact adjust effectively the PHGCs.

Table VII presents the core analysis results whose mesh refinement is same as that in the generation of SPH factors. It is clearly shown that the SP_3 shows better accuracy than diffusion with 8x8 sub-meshes and corresponding SPH factors rather than the 1x1 structure.

Table VII: Core analysis results varying mesh refinement

ID	SPHINCS discretization		$\Delta\rho$ (pcm)	ΔP (Max.)	ΔP (RMS)
Unrodded	1x1	D	-23.4	-1.98	0.65
		SP_3	20.6	-4.08	1.43
	8x8	D	-10.7	3.12	0.86
		SP_3	34.1	-1.27	0.55
Rodded-A	1x1	D	-173.8	-4.15	1.47
		SP_3	-98.2	-6.93	1.43
	8x8	D	-70.9	4.52	1.30
		SP_3	-0.9	1.97	0.60
Rodded-B	1x1	D	-198.4	-8.16	2.39
		SP_3	-97.0	-10.9	2.05
	8x8	D	-85.1	3.80	1.89
		SP_3	15.1	2.73	0.67

4. Conclusion

Among the four errors in the two-step method, the degree of transport and discretization errors were assessed. The deviation of SPH factors was used to measure the degree of correction introduced by the SPH method for both the diffusion and SP_3 FDM solver varying mesh refinement. In cases that the discretization error is sufficiently reduced, the correction effect of SPH is smaller in the SP_3 than the diffusion. In addition, the core calculation results with different mesh size reveals that the SP_3 is fundamentally more accurate than the diffusion but the use of fine mesh is essential,

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