Preliminary Development of Simplified P_3 based Pin-by-pin Core Simulator, SPHINCS

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1. Introduction

Although the recent trend in the development of reactor analysis methods is to enhance accuracy of solution, there is still a preference for two-step core calculation system especially in the reactor design and analysis because of its computational efficiency. Conventionally, assembly-wise two-step core analysis has been performed throughout nTRACER-RENUS core analysis system. nTRACER [1], direct whole core transport code, is used to generate sets of group constants and corresponding reference solution. With those sets of group constants which is generated throughout assembly-wise homogenization and simple energy group condensation, RENUS [2] performs core analysis based on efficient nodal methods which is very fast yet guarantee appropriate bias and uncertainties.

However, increasing the code accuracy has been strongly required in order to obtain additional calculation margins which would be beneficial in regulations related to the safety of core design. Conventional assembly-wise two-step core calculation system has fundamental weakness depicting change of neutron spectrum according to the surrounding loading pattern. Therefore, in the process of generating group constants, pin-wise homogenization and increasing the number of energy is done in order to overcome this weakness. Also, apart from conventional diffusion theory, simplified Pn method is introduced. Especially SP_3 method is well known as a great solution compared with diffusion equation since its formulation is similar so that it has advantage in implementation as well as not a big computational burden. In addition to that, SP_3 method has merit where there appear large spatial neutron flux variation such as MOX fuel loaded cases or control rod insertion cases.

In this regard, the SPHINCS (Simplified P_3 Pin Homogenized Innovative Neutronic Core Simulator) code has been developed at Seoul National University as an improved two-step core calculation system. In this paper, preliminary development of efficient and accurate pin-by-pin core analysis system is introduced.

2. Development Strategy for SP_3 based Pin-by-pin Core Simulator

Considering the scale of geometry, pin-by-pin core analysis code is developed based on SP_3 employing pin-wise finite difference method (FDM), while conventional assembly-wise two-step core analysis system employs various kinds of nodal methods. The typical length of pin pitch is quite long to apply FDM directly but the usage of super homogenization method can compensate inaccuracy.

2.1. Application of Super Homogenization Method

As a first part of two-step core analysis, heterogeneous structure inside the single fuel assembly is homogenized into pin-wise group constants. In the conventional assembly-wise homogenization, neutron balance equation for each assembly should be valid since assembly-wise homogenized XSs preserve all kinds of reaction rates and all net currents are zero at the assembly interface. However apart from that, in pin-wise homogenization, the neutron balance would not be preserved in each pin boundary as the spatial homogenization is done. Due to these reduction of scale, Super homogenization (SPH) method [3] is introduced in order to reduce pin-homogenization error. The SPH factor is generated through iterative procedure which makes homogeneous solution same to the heterogeneous solution while preserving the reaction rate of each pin and is incorporated into the sets of cross section themselves.

From heterogeneous geometry calculation, reference solution is obtained and the reaction rate obtained by homogenized group constants is not conserved compared with reference solution. Therefore introduce SPH factor and adjust homogenized group constants to preserve reaction rate as follows.

$$\bar{\Sigma}_m \bar{\phi}_m \neq \bar{\Sigma}_m \bar{\phi}_m^*, \quad \varsigma = \frac{\bar{\phi}_m^*}{\bar{\phi}_m}$$
$$\varsigma \bar{\Sigma}_m \bar{\phi}_m = \bar{\Sigma}_m \bar{\phi}_m^* \tag{1}$$

Throughout iterative procedure, SPH factors of every pin are converged so that all the reaction rates are preserved.

The necessity of a SPH factor is examined using a sets of typical PWR fuel assembly which consists of a 16x16 array of 236 fuel rods and 5 guide tubes, which displace 4 fuel rod positions respectively.

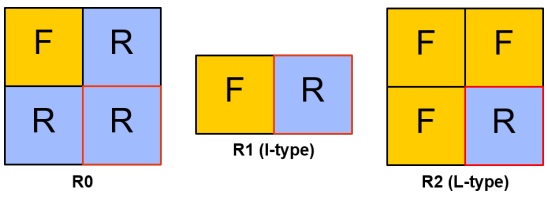

Fig. 1. Fuel-reflector configuration for the generation of radial reflector XSs.

Table I: 2D assembly analysis without SPH factors

Asm. ID	nTRACER	w/o SPH	Δρ (pcm)
A0	0.98226	0.98198	-29
B0	1.18288	1.28252	-26
B1	1.01296	1.01803	493
B2	1.00124	1.00644	516
B3	0.96640	0.97243	642
C0	1.21558	1.21527	-21
C1	1.06297	1.06744	394
C2	1.01870	1.02395	503
C3	1.00798	1.01335	526
R0	0.88271	0.88484	272
R1	1.03138	1.03300	153
R2	1.11309	1.11416	86

As shown in Table I, unless SPH factors are considered, there was a large reactivity discrepancy due to pin-wise spatial homogenization errors. However when converged SPH factors are used, k-effective and pin power distribution become exact same as nTRACER. Those SPH factors are incorporated into cross sections and are used in core calculations.

2.2. SP_3 based 2D-1D Synthesis Method with Transverse Leakage

2D-1D synthesis method is one of the widely used methods for 3D core analysis such as the synthesis of 2D radial calculation by Method of Characteristics (MOC) with 1D axial calculation by nodal method. SPHINCS also employs 2D-1D synthesis method in order to solve 3D problem efficiently. Plane-wise radial calculation is done with pin-wise FDM and axial calculation is done for every pins with fine-mesh FDM. The transverse integrated one-dimensional SP_3 equations are given as:

$$\begin{bmatrix} -D_{0,g}\frac{d^2}{dx^2}+\Sigma_{r,g} & -2\Sigma_{r,g} \\ -\frac{2}{3}\Sigma_{r,g} & -D_{2,g}\frac{d^2}{dx^2}+\frac{4}{3}\Sigma_{r,g}+\frac{5}{3}\Sigma_{t,g} \end{bmatrix} \begin{bmatrix} \hat{\phi}_g^{(0)} \\ \phi_g^{(2)} \end{bmatrix} = \begin{bmatrix} q_g^{(0)}-L_0 \\ -\frac{2}{3}q_g^{(0)}-L_2 \end{bmatrix} \quad (2)$$

where q, L_0 and L_2 on the right hand side are the source and transverse leakage terms corresponding to the scalar flux and second order angular moment.

Alternating direction calculation scheme is implemented throughout using transverse leakage terms. Axial transverse leakage terms and radial transverse leakage terms are applied in the following radial source terms and axial source terms respectively. As the alternating direction calculation iteratively performed, converged solution is obtained.

2.3. Functionalization of Group Constants and Pin-wise T/H Feedback Capability

For hot full power calculations or the cases with T/H feedback and depletion, sets of group constants should be tabulated in terms of branch conditions. Therefore functionalization of effective XSs are performed in SPHINCS about conventionally used variables for branch conditions such as burn-up, fuel temperature, moderator temperature and boron concentration. Functionalization is based on following equation.

$$\begin{aligned} &\sigma\left(BU, ppm, T_f, T_m\right) \\ &= \sigma\left(BU, ppm_0, T_{f0}, T_{m0}\right) \\ &+ \frac{\partial\sigma}{\partial ppm}\left(ppm - ppm_0\right) + \frac{\partial\sigma}{\partial\sqrt{T_f}}\left(\sqrt{T_f} - \sqrt{T_{f0}}\right) \\ &+ \frac{\partial\sigma}{\partial T_m}\left(T_m - T_{m0}\right) \end{aligned} \quad (3)$$

In the process of branch calculation, group constant treatment with SPH factors is important. Since SPH factors are incorporated in initial state, base condition XS sets for branch calculations are no more "base" condition. Consequently SPH factors should be generated for all the branch conditions. Following table shows the effect of incorporating SPH factors in functionalization of group constants.

Table II: SPHINCS results compared with nTRACER according to the existence of SPH factors

C0. HFP. T/H on.	Without SPH	With SPH
k-effective	1.31592	1.31776
Δρ (pcm)	-66	40
Diff. Max. Pin. Pow. [%]	1.10	-0.08

After SPH factors are incorporated for branch conditions, both reactivity and pin power discrepancy decreased a lot. Whether considering SPH or not shows 106pcm reactivity difference and maximum 1.16% pin power difference for each other even though it is single assembly problem.

2.4. Pin-wise Depletion Capability

For a reactor core design, there is a need for depletion calculation capability and apart from steady state calculation, material composition and corresponding isotope number density becomes changed. Therefore microscopic XSs and corresponding sets of isotope number density should be properly considered in depletion calculation.

In SPHINCS, pin-wise depletion module is implemented with 70 nuclides with 4 fissile nuclides while 19 nuclides with 4 fissile nuclides are used for steady state calculation.

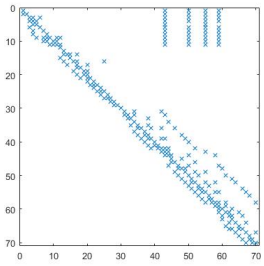

Fig. 2. Burn-up matrix used in SPHINCS.

In conventional assembly-wise nodal two-step calculation, linear depletion method [4] is widely used. Even though it has advantage that analytic solution can be obtained, linear chain structure has fundamental weakness. There is clear drawback that possibility which induces recursive chain such as (n,2n), (n,α) exists and those can't be depicted properly through linear chain.

$$\frac{dX_i(t)}{dt} = \sum_{\substack{j=1 \\ j\neq i}}^{N} l_{ij}\lambda_j X_j + \bar{\phi}\sum_{\substack{j=1 \\ j\neq i}}^{N} \gamma_{ij}\sigma_j X_j - \left(\lambda_i + \sigma_i\bar{\phi}\right)X_i \tag{4}$$

From this reason, in SPHINCS, Krylov subspace expansion method [5] is used to solve matrix exponential problem.

$$\frac{d\vec{X}(t)}{dt} = A\vec{X}_0,\ \vec{X}_1 = \exp\left(A\Delta t\right)\vec{X}_0 \tag{5}$$

Since the SPH factor is defined as a ratio of heterogeneous flux to homogeneous flux and is introduce in order to preserve reaction rate, Bateman equation also should be treated properly with SPH factors. Similar to the point as mention in Section 2.3, SPH update should be performed for all the burn-up steps (i.e. branch conditions). Isotope number density is obtained using flux and the flux should be "true flux" incorporated with SPH factors. Following is true flux obtained by the definition of SPH factor.

$$\bar{\phi}_m^* = \zeta\bar{\phi}_m \tag{6}$$

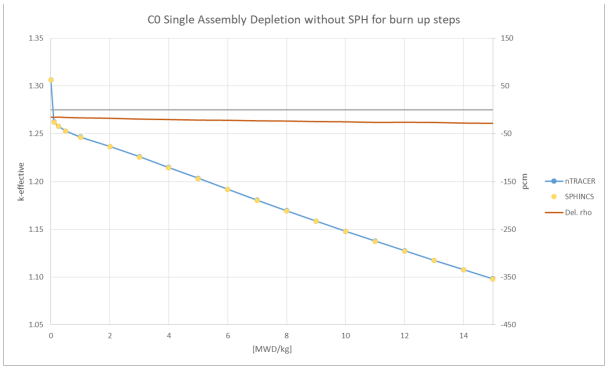

Fig. 3. Consistent under-estimation of k-effective without SPH updates.

Unless SPH factors are updated in all the burn-up steps, consistent large under-estimation of k-effective is shown through all the steps as shown in Fig. 3.

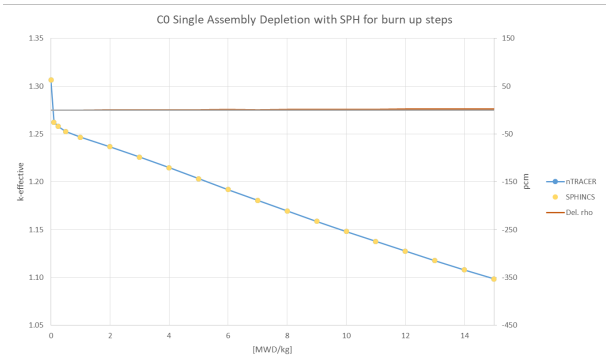

Fig. 4. Depletion results of SPHINCS with SPH update.

Large discrepancy of k-effective is resolved with properly generated SPH factors so that depletion result of SPHINCS show great agreement compared with that of nTRACER.

3. Numerical Results

With properly generated SPH factors, functionalization of XSs, T/H feedback and depletion capability is implemented in SPHINCS which employs 2D-1D synthesis method with transverse leakage. Fig. 5 shows schematic diagram of SPHINCS code structure.

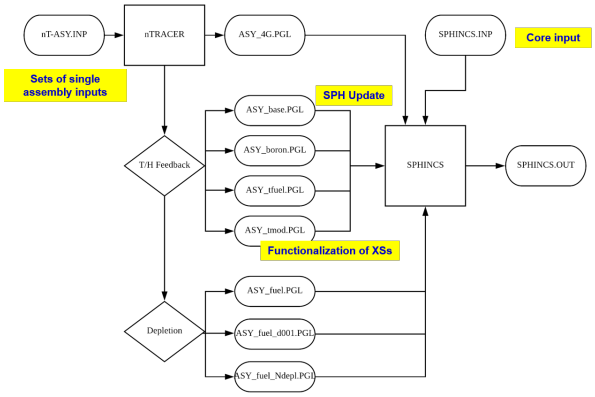

Fig. 5. Schematic diagram of the SPHINCS system.

The numerical results shown in this section are mainly focused on two parts. One is the verification of alternating direction scheme itself and the other is core calculation results.

3.1. Verification of 2D-1D Synthesis Method

C5G7 benchmark problems (Benchmark on Deterministic Transport Calculations Without Spatial

Homogenization) [6] are used for verification of the calculation scheme as well as strength of SP_3 method rather than diffusion method. For a given C5G7 benchmark XSs, nTRACER generates reference solution and pin homogenized group constants. Both SP_3 and diffusion calculation options of SPHINCS are compared with nTRACER.

Table III: Comparison of both calculation modules in SPHINCS for C5G7 3D assemblies

Description	nTRACER	SPHINCS		SPHINCS-D	
UO_2	1.28217	1.28204		1.28183	
		-8		-21	
Pin power diff. RMS/Max [%]		0.00	0.01	0.01	0.16
MOX	1.14459	1.14477		1.14317	
		14		-109	
Pin power diff. RMS/Max [%]		0.00	0.03	0.20	0.93

As shown in Table III, both SP_3 and diffusion modules of SPHINCS employing alternating direction calculation scheme show great agreement compared with nTRACER. For UO_2 assembly case, there is not much difference between two options in aspect of reactivity and pin power difference. Contrary to that, for MOX assembly case, the strength of employing SP_3 is clearly shown.

3.2. Checkerboard & Quarter Core Analysis

Two of the assemblies mentioned in Section 2.1 were chosen to construct checkerboard problem. For 2D quarter core analysis, APR1400 problem is constructed. Group constants are generated based on single assembly by nTRACER and the number of energy group is 8G.

Table IV: Results of checkerboard and core analysis.

Description	nTRACER	SPHINCS (8G)	
A0/C2 Checkerboard	1.02728	1.02723	
		-5	
Pin power diff. RMS/Max [%]		0.33	-0.83
2D Quarter Core	1.01410	1.01430	
		20	
Pin power diff. RMS/Max [%]		0.40	-1.40

Fig. 6. Absolute pin power difference of 2D quarter core.

As shown in Table IV and Fig. 6, SPHINCS shows great agreement compared with nTRACER for both checkerboard and quarter core problems in aspect of k-effective and pin power distribution.

4. Conclusion

As an improved two-step core calculation system, preliminary development of the SPHINCS code which is SP_3 based pin-by-pin neutronic core simulator has been done. Apart from conventional assembly-wise homogenization based nodal method, pin-wise homogenization with properly generated SPH factors is introduced with a few energy group structure. Alternating direction calculation scheme is applied as a synthesis of radially pin-wise FDM with axially fine-mesh FDM. 2D-1D synthesis method of SPHINCS employing SP_3 based FDM shows great agreement with nTRACER. Also for the case that has large spatial flux variation, SP_3 shows strength than diffusion.

Pin-wise T/H feedback capability as well as pin-wise depletion capability have been implemented in SPHINCS. While performing feedback and depletion, SPH factors also should be considered properly. With properly generated SPH factors, SPHINCS works well for feedback or depletion conditions compared with nTRACER.

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