Analysis of Pressurized Water Reactor Pin-by-pin Homogenization

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ABSTRACT

Homogenization performances for pin cells in 2D geometry are analyzed in order to facilitate pin-by-pin core calculation. There are different choices for spatial homogenization, energy homogenization and the corresponding core calculation methods. Two spatial homogenization methods were investigated including the generalized equivalence theory (GET) and the super-homogenization (SPH) method. Energy groups were condensed from the 69 WIMS-D4 structure to either 2 or 7 together with spatial homogenization. Both P₁ and SP₃ were employed as pin-homogenized core calculation methods. The pin-homogenized core calculation results were compared with the original heterogeneous core calculation. In addition, the traditional two-step calculation with assembly homogenization and pin-power reconstruction was employed as a comparison. The numerical results revealed encouraging conclusions. (1) The pin-by-pin calculation scheme can provide more accurate results than the traditional two-step calculation. (2) Different spatial homogenization techniques can provide results with similar accuracy. (3) Energy groups has to be increased together with spatial homogenization zone refinement.

Key Words: Homogenization, pin-by-pin, Generalized Equivalence Theory, SPH.

1. INTRODUCTION

For Pressurized Water Reactor (PWR) neutronics calculation, direct treatment of detailed structure in actual three-dimensional geometry [1] is unacceptable for routine calculation so far mainly due to the computing time and storage requirement. Thus, traditionally PWR is calculated based on the so-called two-step approach [2], which consists of lattice homogenization, few-group constant parameterization, reactor core diffusion calculation and pin-power reconstruction. The heterogeneous structure within each assembly is homogenized into a single or four regions. This scheme is very efficient and requires only a small amount of memory. Thus, the assembly homogenization methods have been developed along with the two-step calculation.

Advanced nodal methods [3] are widely used in reactor analysis and design nowadays along with the homogenization method and the pin power reconstruction techniques. There are many homogenization methods for fuel assemblies proposed. The most popular method is the generalized equivalence theory (GET) developed by Smith [4], which is based on the equivalence theory proposed by

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Koebke [5]. One of the significant features of GET is that the assembly homogenization parameters (i.e. assembly discontinuity factors, ADF) are obtained from the single assembly calculation with a reflective boundary condition [6]. Regardless to the locations of the fuel assemblies, the same assembly type has the same homogenization parameters.

The traditional two-step calculation scheme needs two homogenizations respectively in pin-cell and assembly levels to obtain single or quarter assembly homogenized few-group constants. The core calculation also requires pin-power reconstruction techniques to obtain the pin-power distribution which is important for safety analysis. With the development of computing technology, an alternative scheme [7] with more detailed core modeling named pin-by-pin calculation [8] becomes attractive in recent years. Heterogeneous structure in pin cells (i.e. pellet, clad and moderator) is homogenized into a node and a pin-by-pin whole core simulator is employed. The pin-by-pin calculation scheme eliminates the assembly homogenization and the pin power reconstruction to provide better precision with a reasonable cost.

The most significant feature between the pin-cell and the assembly homogenizations is the different optical thickness of the homogenized region. The size of a pin cell is much smaller than that of an assembly, resulting that the homogenization parameters of the pin cell being more environments dependent. The surroundings of each pin cell will strongly affect the target pin, especially when the target pin is adjacent to pin cells like strong absorbers. The interference effect is much stronger for pin cells when different types of fuel pins are adjacent. So the single pin cell calculation for pin-cell homogenization just like the single assembly calculation for assembly homogenization can bring in a large error and hence unacceptable. In order to reduce the error of the cell-level homogenization, cell heterogeneous calculation in a larger geometry should be carried out. During the past decade, pin-cell heterogeneous assembly calculations were getting in practical use [9]. And several pin-cell homogenization methods [10] have been developed for the pin-cell homogenization on the assembly-level heterogeneous calculation.

There are two popular homogenization methods for the pin-cell homogenization. The first one is the super homogenization (SPH) method. It is proposed by Kavenoky [11] and then developed by Hebert to the pin-cell homogenization [12]. After that, Yamamoto and Tastumi applied the method to the SCOPE2 [13]. The other one is the generalized equivalence theory. The pin discontinuity factors [14] (PDF) or the current discontinuity factors [15] (CDF) were proposed to be applied in the pin-cell homogenization.

Focused on the homogenization technology, this paper analyzed the GET and the SPH method applied to pin-cell levels homogenization. And different energy-group structures will be tested in a typical 2D PWR core problem. The core calculation method is optional between diffusion or SP₃ method. The reference solution will be obtained by the multi-group heterogeneous core calculation with transport code. What's more, the two-step calculation will also be carried out as a comparison to determine how much precision can be improved. The influence affected by the reflective boundary conditions will also be analyzed quantitatively.

2. METHOD

This section provides an introduction of the GET and the SPH method aiming at both P1 and SP₃. Different energy-group structures would not change the formulas, so the energy-group structure is not discussed in this section.

2.1. The Generalized Equivalence Theory (GET)

It was proposed by Koebke in 1970s [5]. An interface relationship between the nodes was introduced to preserve the integral reaction rate within each node and the leakage rate on each interface. The homogeneous surface flux would be continuous via the equivalence factors which are the original discontinuity factors. After that, Smith developed the GET in routine calculation [4].

The discontinuity factor is defined as the ratio of the heterogeneous over the homogeneous surficial fluxes:

$$f_{s,i,g} = \frac{\phi_{i,g}^{s,het}}{\phi_{i,g}^{s,hom}} \tag{1}$$

where, subscript *s*, *i* and *g* stand for the surface, the node and the energy group. $\phi_{i,g}^{s,het}$ (cm⁻²·s⁻¹) is the nodal surface flux obtained from pin-heterogeneous neutron transport calculation together with the nodal surface net current $J_{i,g}^{s,het}$ (cm⁻²·s⁻¹) and the nodal volumetric averaged flux $\overline{\phi}_{i,g}^{het}$ (cm⁻²·s⁻¹); in contrast, $\phi_{i,g}^{s,hom}$ (cm⁻²·s⁻¹) is the nodal surface flux which is supposed to be obtained from the homogeneous neutron diffusion calculation.

Consequently, the point is how to estimate the homogeneous surface flux accurately before the homogeneous calculation.

2.1.1. The assembly GET

For the assembly homogenization, in order to preserve the integral reaction rate inside a node, the nodal volumetric averaged flux of the homogenization calculation should be equal to that of the heterogeneous calculation. Due to the reflective boundary condition adopted in the single assembly calculation, the nodal surface flux obtained from the homogenization calculation should be equal to the nodal volumetric averaged flux

$$\phi_{i,g}^{s,\text{hom}} = \overline{\phi}_{i,g}^{\text{het}} \tag{2}$$

2.1.2. The pin-cell GET

In contrast, for the pin-by-pin homogenization, to get rid of the non-linear relationship between the homogeneous surficial flux and the pin discontinuity factors (PDF), the flux distribution approxi-

mation for the homogeneous surficial flux has to be exactly the same as the actual following homogeneous core calculation. In this paper, the Exponential Function Expansion Nodal method (EFEN) [16] was employed for both the homogeneous diffusion (P_1) and SP_3 core calculation.

In the EFEN diffusion method, we can get the partial current response relation via the undetermined coefficient method with the constraints for net currents surface fluxes and node-average flux:

$$J_{x+,i,g}^{hom,out} = \mu_{x,i,g}^{hom} J_{x+,i,g}^{hom,in} + \eta_{x,i,g}^{hom} \overline{\phi}_{i,g}^{hom} + \xi_{x,i,g}^{hom} S_{i,g}^{'}$$

$$(3)$$

$$S_{i,g}^{'hom} = S_{i,g}^{hom} - \frac{J_{y+,i,g}^{hom} + J_{y-,i,g}^{hom}}{h_{i,y}} - \frac{J_{z+,i,g}^{hom} + J_{z-,i,g}^{hom}}{h_{i,z}}$$
(4)

where, subscript x, y, z stand for the coordinates, h is the nodal dimension (cm), coefficients $\mu_{x,i,g}^{hom}$, $\eta_{x,i,g}^{hom}$, $\xi_{x,i,g}^{hom}$ are determined by the cross sections and the nodal dimensions, the $S_{i,g}^{hom}$ refers to the sum of the scattering source from other energy groups and the fission source from all the energy groups, $J_{i,g}^{hom}$ is the net currents (cm⁻²s⁻¹).

According to the Fick's low, the relationship between the partial current, the net current and the surficial flux is as following:

$$\begin{cases} \phi_{x\pm,i,g}^{s,hom} = 2\left(J_{x\pm,i,g}^{hom,out} + J_{x\pm,i,g}^{hom,in}\right) \\ J_{x\pm,i,g}^{hom} = J_{x\pm,i,g}^{hom,out} - J_{x\pm,i,g}^{hom,in} \end{cases}$$
(5)

Substituting Eq. (3) into Eq. (5), the homogeneous nodal surface flux can be expressed as the following:

$$\phi_{x\pm,i,g}^{s,hom} = \frac{2}{\left(\mu_{x,i,g}^{hom} - 1\right)} \left[\left(\mu_{x,i,g}^{hom} + 1\right) J_{x\pm,i,g}^{hom} - 2\eta_{x,i,g}^{hom} \overline{\phi}_{i,g}^{hom} - 2\xi_{x,i,g}^{hom} S_{i,g}^{'hom} \right]$$
(6)

Since the volumetric flux and the surface net current should be preserved during the homogenization process, the homogeneous quantities can be replaced by the corresponding heterogeneous ones.

$$\phi_{x\pm,i,g}^{s,hom} = \frac{2}{\left(\mu_{x,i,g}^{hom} - 1\right)} \left[\left(\mu_{x,i,g}^{hom} + 1\right) J_{x\pm,i,g}^{het} - 2\eta_{x,i,g}^{hom} \overline{\phi}_{i,g}^{het} - 2\xi_{x,i,g}^{hom} S_{i,g}^{'het} \right]$$
(7)

For the EFEN SP₃ method, different from EFEN diffusion or SP₁, it contains a 2^{nd} order flux moment as shown in the following Eqs.:

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$$\begin{cases} -D_{1}\nabla^{2}\varphi_{0} + \Sigma_{r}\varphi_{0} = s_{0} + 2D_{1}\nabla^{2}\varphi_{2} \\ -\frac{11}{7}D_{1}\nabla^{2}\varphi_{2} + \Sigma_{tr}\varphi_{2} = \frac{2}{5}D_{1}\nabla^{2}\varphi_{0} \end{cases}$$
(8)

Through the same derivation as that in the EFEN diffusion method, the homogeneous nodal surficial flux can be obtained as following:

$$\begin{cases} \varphi_{x+,i,g}^{0,sur,hom} = \frac{2}{\left(\mu_{x,i,g}^{0,hom} - 1\right)} \left[\left(\mu_{x,i,g}^{0,hom} + 1\right) J_{x+,i,g}^{0,het} - 2\eta_{x,i,g}^{0,hom} \left(\overline{\varphi}_{i,g}^{0,het} + 2\overline{\varphi}_{i,g}^{2,het}\right) - 2\xi_{x,i,g}^{0,hom} S_{i,g}^{(1,het)} \right] \\ \varphi_{x+,i,g}^{2,sur,hom} = \frac{2}{\left(\mu_{x,i,g}^{2,hom} - 1\right)} \left[\left(\mu_{x,i,g}^{2,hom} + 1\right) J_{x+,i,g}^{2,het} - 2\eta_{x,i,g}^{2,hom} \overline{\varphi}_{i,g}^{2,het} - 2\xi_{x,i,g}^{2,hom} S_{i,g}^{(2,het)} \right] \end{cases}$$
(9)

The single assembly heterogeneous neutron transport calculation is usually done by a high order angular approximation method such as MOC or Sn which can provide the heterogeneous value of $\overline{\varphi}_{i,g}^{0,het}$ and $J_{x+,i,g}^{0,het}$ but not the 2nd order flux moment. There are several approaches to obtain the 2nd order flux moment. One can reconstruct it by using the SP₃ theory proposed by Chao-Yamamoto [17]. Or one can just simply solve the second Eq. of the SP₃ equations by constructing the source term which is the leakage of the scalar flux. In this work, a pseudo fixed source problem [18] was employed:

$$-\frac{11}{7}D_{1,i,g}\nabla^2 \varphi + \Sigma_{tr,i,g}\varphi_{2,i,g}^{hom} = s_{i,g}$$
(10)

$$s_{i,g} = \frac{2}{5} D_{1,i,g} \nabla^2 \varphi_{0,i,g}^{het}$$
(11)

However, the PDF for the 2nd order flux still cannot be obtained even with the heterogeneous and homogeneous φ_2^{sur} known. Different from φ_0 , the value of φ_2^{sur} is small or even negative, which may yields very large or even negative PDF if the definition of the 2nd order flux has the same form as that of the scalar flux. Unfortunately, negative PDFs may cause the divergence of the EFEN SP₃ solution iteration. To avoid that from happening, the definition of PDF for the 2nd order flux.

$$f_{2,i,g}^{s} = \frac{\varphi_{2,i,g}^{s,\text{het}} + \Delta \varphi_{2,i,g}}{\varphi_{2,i,g}^{s,\text{hom}} + \Delta \varphi_{2,i,g}}$$
(12)

And then instead of Eq. (10), the flowing Eq. is solved as the pseudo fixed source problem.

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$$-\frac{11}{7}D\nabla^2\varphi_2 + \Sigma_{tr}\left(\varphi_2 + \Delta\varphi_2\right) = \frac{2}{5}D\nabla^2\varphi_0 + \Sigma_{tr}\Delta\varphi_2 \tag{13}$$

2.2. The Super Homogenization Method (SPH)

Its basic idea is to preserve the reaction rate through the cross sections corrected by a set of correction factors called SPH factors.

$$\overline{\Sigma}_{x,i,g}^{SPH} \int_{r} \phi_{i,g}^{hom} dv = \overline{\Sigma}_{x,i,g} \int_{r} \phi_{i,g}^{het} dv$$

$$(14)$$

$$\Sigma_{x,i,g}^{STI} = \mu_{i,g} \Sigma_{x,i,g} \tag{15}$$

Substituting Eq. (15) into Eq. (14) yields the definition of the SPH factor:

$$\mu_{i,g} = \frac{\overline{\phi}_{i,g}^{het}}{\overline{\phi}_{i,g}^{hom}} \tag{16}$$

where, $\overline{\Sigma}_{x,i,g}$: the average cross section via the flux volume weight method (FVW); $\overline{\phi}_{i,g}^{het}$: the average neutron flux from the cell heterogeneous calculation; $\overline{\phi}_{i,g}^{hom}$: the average neutron flux obtained by the cell homogenization calculation with the SPH corrected cross section.

In the SPH method, the following normalization of the neutron fluxes has been performed:

$$\overline{\phi}_{i,g}^{hom,norm} = \overline{\phi}_{i,g}^{hom} \frac{\sum\limits_{g' \in g} \sum\limits_{k} \phi_{k,g}^{het} V_k}{\sum\limits_{i} \overline{\phi}_{i,g}^{hom} V_i}$$
(17)

where $V_i = \sum_{k \in i} V_k$: Volume of the homogenized node.

It is an iterative calculation to obtain the SPH factors. In the iterative calculation, the cell homogenization calculation method (EFEN) used has to be exactly the same with the active following core calculation.

- The calculation strategy contains four steps: 1. Solve the heterogeneous problem to get $\overline{\phi}_{i,g}^{het}$ and $\overline{\Sigma}_{x,i,g}$;
- 2. Set the SPH factors to the initial values;
- 3. Solve the homogeneous problem to get $\overline{\phi}_{i,g}^{hom}$ and then the updated SPH factor;
- 4. Correct the cross sections and check if the SPH factors are convergent. If not, go back to step 3.

The differences between the SPH methods in EFEN diffusion and SP₃ method is the target homogenization parameters which would be corrected by the SPH factors. In the EFEN diffusion method, the absorption cross section, the fission and scatter cross section together with the diffusion coefficient should be involved in the correction, while the total cross section, the fission and the scatter cross section in the EFEN SP₃ method.

3. NUMERICAL RESULTS

3.1. Verification of the Pin-cell Homogenization Methods

Two single assembly problems with reflective B.C. respectively w and w/o burnable absorbers were tested. Their configurations are showed in Fig. 1 and Fig. 2. There are 17x17 pin cells in each assembly. The white, gray and orange pin represents the fuel rod, guide tube and gadolinium rod (Gd rod) respectively. Each heterogeneous pin cells consist of pellet, cladding and moderator. The geometry of the pin cell and the material filled in the assembly are showed in Table 1.



Fig. 1 PWR assembly without Gd rod



Fig. 2 PWR assembly with 12 Gd rods

Geometry	Value	material	Value
Pellet Radius	0.4096 cm	Fuel: UO ₂	3.1% (enrichment)
Inner Clad Radius	0.418 cm	Cladding	Zircaloy-nat
Outer Clad Radius	0.475 cm	Moderator	water
Rod Pitch	1.26 cm	Gd rod: UO2-Gd2O3	3.1% UO ₂ ; 9% Gd ₂ O ₃

Table 1 Geometry and material for pin cells

The results in Table 2 indicate that the heterogeneous problem with reflective B. C. can be recovered by either the GET or SPH method, including the eigenvalue and the pin cell integral reaction rates.

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Energy	Angular treatment	Homogenization Method	Assembly without Gd		Assembly With 12 Gd	
groups			<i>k_{eff}</i> (pcm)	Pin power	<i>k_{eff}</i> (pcm)	Pin power
				max error		max error
2	Diffusion	GET	0	0.01%	0	0.01%
		SPH	3	0.01%	2	0.01%
	SP ₃	GET	0	0.01%	1	0.01%
		SPH	2	0.01%	3	0.01%
7	Diffusion	GET	1	0.01%	0	0.01%
		SPH	3	0.01%	1	0.01%
	SP ₃	GET	0	0.01%	1	0.01%
		SPH	2	0.01%	0	0.01%

Table 2 Results of the single-assembly calculations

3.2. Evaluation of the Homogenization Methods

A two-dimensional 1/4 PWR core as showed in Fig. 3 was employed to evaluate the following homogenization methods:

- (1) The heterogeneous reference solution provided by, a MOC code.
- (2) Single assembly calculations with reflective B. C. determine the 2-groups assembly homogenization parameters including the assembly discontinuity factors (ADF), followed by the core diffusion calculation and the pin-power reconstruction. This is the legacy scheme.
- (3) Single assembly calculations with reflective B.C. determine the pin-cell homogenization 2-groups/7-groups parameters including the PDF and the cross section corrected by the SPH factors, followed by the core diffusion/SP₃ calculations. These are the pin-by-pin schemes.

The core consists of 3.65% UO₂ and 4.95% UO₂ assemblies. The number *N* appeared in each node represent the number of the Gd rods in the assembly. The Gd enrichment is 0.71% if *N* is less than 20, while the other is 2.5%. Every assembly consists of 17x17 pin cells, the cell-pitch is 1.26 cm and the water gap is 0.042 cm, thus the center distance of the assembly is 21.504 cm.

As in Table 3, the numerical results indicate that compared with the two-step calculation, the pin-by-pin calculations with 2-groups structure have a larger error, no matter the pin-cell homogenization method is the GET or the SPH method, while the 7-groups structure will lead to a good result. This is due to the stronger spectral interference in the pin-by-pin calculation. The reference pin-power distribution is showed in Fig. 4 and the error of the reconstructed pin power of two-step calculation is showed in Fig. 5. The maximum error appeared in Fig.5 is in the corner of the assembly which is adjacent to the reflector and the value is about 20%. Except these pins, the max error is about 13%.

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Fig. 3 The configuration of the 1/4 PWR core

Table 5 The eigenvalue results of the two-dimensional F with broblen

Case	Energy Groups	Angle	$k_{e\!f\!f}$	Difference(pcm)
Reference	69	MOC	1.25736	-
Two-step(ADF)	2	P1	1.26160	424
Pin-by-pin(PDF)	2 7		1.26599	863
Pin-by-pin(SPH)		P1	1.26126	390
Pin-by-pin(PDF)			1.25716	-20
Pin-by-pin(SPH)			1.25832	96
Pin-by-pin(PDF)	2	SP ₃	1.26616	880
Pin-by-pin(SPH)			1.26147	411
Pin-by-pin(PDF)	7		1.25711	-25
Pin-by-pin(SPH)			1.25869	133

As shown in Fig. 6, the results indicate that diffusion calculation or the SP₃ calculation utilized with the SPH factors is better than the calculation with PDFs, the max error of the PDF and that of the SPH are very close. However, no matter which pin-cell homogenization method is used, the pin-by-pin calculation with 2-groups structure is worse than the two-step calculation.

PHYSOR 2016 – Unifying Theory and Experiments in the 21st Century Sun Valley Resort, Sun Valley, Idaho, USA, May 1 – 5, 2016, on CD-ROM (2016)



Fig. 4 The reference pin-power distribution



Fig. 5 Relative pin-power error of two-step calculation



Fig. 6 Relative pin-power error of the pin-by-pin calculation, (a) the 2G diffusion calculation with PDF, (b) the 2G SP₃ calculation with PDF, (c) the 2G diffusion calculation with SPH factor, (d) the 2G SP₃ calculation with SPH factor

As in Fig. 7, the pin-power error of the pin-by-pin calculation with 7-group structure indicates that either the diffusion or SP₃ calculation with 7-groups structure is more accurate than the two-step calculation. And the SP₃ calculation is better than the diffusion calculation, no matter which homogenization method is utilized. Except the corner locations adjacent to the reflector, the maximum pin-power error is about 7% for the diffusion calculation and 5% for the SP₃ calculation. The big

errors always appear in the boundary of an assembly, especial the corners. Because the pin-cell homogenization parameters (i.e. discontinuity factors or SPH factors) are generated in single assembly calculation with a specific boundary conditions (zero current), they cannot exactly correct the homogenization error completely when they come to the core. So there still exists a need to improve these methods to make them less environment dependent.



Fig. 7 Relative pin-power error of the pin-by-pin calculation, (a) the 7G diffusion calculation with PDF, (b) the 7G SP₃ calculation with PDF, (c) the 7G diffusion calculation with SPH factor, (d) the 7G SP₃ calculation with SPH factor

4. CONCLUSIONS

After analyzing different pin-by-pin homogenization techniques and comparing them with the legacy assembly homogenization techniques, this paper provides the following conclusions. (1) Both the GET and the SPH methods work effectively in pin-by-pin calculation scheme. (2) In the two-dimensional PWR core problem, compared with the legacy assembly homogenization technique which causes about 424 pcm errors in k_{eff} and 13.68% maximum pin-power error for the pins which are normal power level, the 7-groups diffusion pin-by-pin homogenization techniques reduces these errors respectively to -20 pcm and 7.53% and 96 pcm and 6.31%, while the 7-groups SP₃ pin-by-pin homogenization techniques reduce these errors respectively to -25 pcm and 5.15% used with the GET and to 133 pcm and 5.37% used with SPH method. (3) For pin-by-pin calculation,

2-groups structure is severely insufficient, while 7-groups have been proved to be sufficient enough. (4) The error brought in by the infinite environment in unit assembly calculation is the main obstacle to improve the accuracy for the PWR core simulator.

In addition, the environment effect was not well treated in this paper. It becomes our next concentration undoubtedly.

ACKNOWLEDGMENTS

This research was carried out under the financial support by the National Natural Science Foundation of China (No. 11305123).

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