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Heterogeneous neutron-leakage model for PWR pin-by-pin calculation

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ABSTRACT

When assembly calculation is performed with the reflective boundary condition, a leakage model is usually required in the lattice code. The previous studies show that the homogeneous leakage model works effectively for the assembly homogenization. However, it becomes different and unsettled for the pin-cell homogenization. Thus, this paper evaluates homogeneous and heterogeneous leakage models used in pin-by-pin calculation. The implements of homogeneous and heterogeneous leakage models used in pin-cell homogenization of the lattice calculation are studied. A consistent method of cooperation between the heterogeneous leakage model and the pin-cell homogenization theory is proposed. Considering the computational cost, a new buckling search scheme is proposed to reach the convergence faster. For practical reactor-core applications, the diffusion coefficients determined by the transport cross-section or by the leakage model are compared with each other to determine which one is more accurate for the Pressurized Water Reactor pin-by-pin calculation. Numerical results have demonstrated that the heterogeneous leakage model together with the diffusion coefficient determined by the heterogeneous leakage model would have the higher accuracy. The new buckling search scheme can decrease the cost dramatically, especially for the heterogeneous leakage model.

1. Introduction

For Pressurized Water Reactor (PWR) core-physics simulation, the computational cost of one-step calculation with fully detailed description is too expensive using either stochastic or deterministic method even with the currently most advanced computing powers. Therefore, the two-step scheme had been developed to provide efficient solutions with an acceptable accuracy. In the last few decades, the nodal diffusion calculation accompanied with the assembly homogenization has been widely employed. The assembly discontinuity factors (ADF) obtained by the generalized equivalence theory (GET) Smith, 1980 is applied. However, neither the axial nor radial leakage rate (Benoist et al., 1994) is considered within the heterogeneous single-assembly calculation. The heterogeneous flux spectrum is far from the actual flux spectrum in the core named global spectrum. The leakage model (Hebert, 2009; Xie, 2001) is then implemented to provide more consistent assembly-homogenized few-group constants and to evaluate depletion process and so on. Moreover, the leakage model is also employed to obtain consistent values of the diffusion coefficient (named leakage coefficient to distinguish with the diffusion coefficient based on transport cross-section) that can be used in three-dimensional full-core diffusion or other low-order calculations. Within the homogeneous leakage model, the heterogeneous assembly is treated as an equivalent homogeneous medium and the axial or radial leakage rate is exactly same under the specific buckling. Thus, it is named as homogeneous leakage model.

As an improved two-step scheme, pin-by-pin calculation has become attractive in recent years (Sugimura et al., 2006; Park et al., 2001). Different from the traditional two-step calculation, it only homogenizes the heterogeneous structure within each pin cell leaving the assembly heterogeneous during the three-dimensional whole-core calculation. Both the Generalized Equivalence Theory and the Super-homogenization (SPH) method have been extended as pin-cell homogenization methods (Zhang et al., 2016). With the reflective boundary condition, either the pin-cell discontinuity factor (PDF) or the SPH factor can fully eliminate the errors aroused by the homogenization once the heterogeneous reference solution is known (Zhang et al., 2016). When the leakage shows up, in either axial or radial direction, a leakage model would be required.

In a PWR core, the effect of scattering anisotropy on the leakage is of prime importance (Hebert, 2009). Therefore, its effect on the leakage model is always taken into account by using a consistent

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B_1 approximation. For the assembly homogenization, a homogeneous consistent B_1 calculation (Stammler and Abbate, 1983) has been proved to be sufficient. Meanwhile, when a leakage model is applied in pin-cell homogenization, the leakage rate will also be affected by the neutron streaming effect (Petrovic et al., 1996). Especially when poison pins or empty channels are present, the streaming effect cannot be ignored anymore. Consequently, the assumption that the neutron flux is homogeneous and the leakage rate is uniform over the lattice pitch is no longer valid. What's more, the leakage model should determine the pin-dependent leakage coefficients for the pin-cell homogenization parameters. In this case, the performance of the homogeneous leakage model is invalid, while a heterogeneous leakage model (Petrovic et al., 1996) becomes a more appropriate choice. In contrast to the homogeneous leakage model assuming spatially constant neutron flux and leakage rate, the heterogeneous leakage model assumes that the neutron flux is variational and the leakage rate is not uniform over the lattice pitch to take into account the characteristics of each pin and the streaming effects within the assembly. In addition, according to the leakage rates of individual pins, the pin-dependent leakage coefficients for the pin-cell homogenization parameters can be determined.

What's more, when the homogeneous leakage model is applied in the lattice calculation for the assembly homogenization, the assembly-homogenized cross-section determined by the flux-volume weight (FVW) method can preserve the eigenvalue and the reaction rate. The global spectrum used to correct the infinite spectrum does not affect the ADF because the same correction appears both in the numerator and dominator in the discontinuity factor calculation. However, for the heterogeneous leakage model in the pin-cell homogenization, there usually are two different spectrum corrections for each interface from the two adjacent pin cells. This effect causes the issue of the cooperation between the heterogeneous leakage model and the pin-cell homogenization method.

In this paper, consequently, both homogenous and heterogeneous leakage models are evaluated for pin-by-pin calculation. Considering the computational cost, three different buckling-search schemes are analyzed, including the legacy power-method scheme, the linear-interpolation scheme and the newly proposed neutron-balance scheme. In addition, the diffusion coefficients obtained from transport cross-section and the space-dependent leakage coefficients from the leakage model are compared for the practical reactor-core pin-by-pin applications.

The rest of this paper is organized as following. Section 2 describes the homogeneous and heterogeneous leakage models and describes their implementations for pin-cell homogenization including three critical buckling search schemes. In Section 3, numerical results for the applications of the leakage models in pin-cell homogenization are analyzed. Finally, Section 4 summarizes the paper. For a better representation, all the abbreviations used in the paper are listed in Table. 1.

Table 1
Abbreviations.

Short forms	Full name	Short forms	Full name
PWR	Pressurized Water Reactor	LC	Leakage Coefficient
ADF	Assembly Discontinuity Factors	DC	Diffusion Coefficient
GET	Generalized Equivalence Theory	W/O	Without
SPH	Super-Homogenization Method	BA	Burnable Absorber
PDF	Pin-cell Discontinuity Factors	2-/7-group	2-Group or/and 7-group
FVW	Flux-Volume Weight Method	Hom	Homogeneous
CBC	Critical Boron Concentration	Het	Heterogeneous

2. Theoratical models

The principle of the neutron-leakage model is to represent the neutron flux as the product of a macroscopic distribution in space $\Psi(\mathbf{r})$ with a fundamental flux $\varphi(\mathbf{r},E,\mathbf{\Omega})$.

$$\phi(\mathbf{r},E,\mathbf{\Omega}) = \Psi(\mathbf{r})\varphi(\mathbf{r},E,\mathbf{\Omega}) \tag{1}$$

The macroscopic distribution $\Psi(\mathbf{r})$ is assumed to be a property of the entire reactor core and to be the solution of a Laplace equation.

$$\nabla^2\Psi(\mathbf{r}) + B^2\Psi(\mathbf{r}) = 0 \tag{2}$$

where the buckling B^2 is a real number that is used to adjust the curvature of $\Psi(\mathbf{r})$ in such a way as to obtain $k_{eff} = k_{eff}^{req}$, where k_{eff}^{req} is the targeted value of k_{eff} which usually is 1.0. In contrast, homogeneous or heterogeneous treatments of the fundamental flux lead to the homogeneous or heterogeneous leakage variants.

2.1. Homogeneous leakage model

In the homogeneous leakage model (Hebert, 2009; Xie, 2001), the neutron flux can be factorized as Eq. (3)

$$\phi(\mathbf{r},E,\mathbf{\Omega}) = \varphi(E,\mathbf{\Omega})e^{i\mathbf{B}\cdot\mathbf{r}} \tag{3}$$

where the parameter $\boldsymbol{B}$ refers to buckling. We note the independence of the fundamental flux $\varphi(E,\mathbf{\Omega})$ with the spatial coordinate.

The neutron-transport equation (Xie and Deng, 2005) for a finite homogeneous geometry is showed as Eq. (4):

$$\mathbf{\Omega}\cdot\nabla\phi(\mathbf{r},E,\mathbf{\Omega}) + \Sigma(E)\phi(\mathbf{r},E,\mathbf{\Omega}) = \int_{4\pi} d^2\Omega' \int_0^\infty dE'\Sigma_s(E \leftarrow E',\mathbf{\Omega}\leftarrow\mathbf{\Omega}')\phi(\mathbf{r},E',\mathbf{\Omega}') + \frac{\chi(E)}{4\pi K_{eff}}\int_0^\infty dE'\nu\Sigma_f(E')\phi(\mathbf{r},E') \tag{4}$$

where

$\Sigma_s(E\leftarrow E',\mathbf{\Omega}\leftarrow\mathbf{\Omega}')$ = macroscopic differential scattering cross-section (cm^{-1})
$\chi(E)$ = fission spectrum
$\Sigma(E)$ = macroscopic total cross-section (cm^{-1})
$\nu\Sigma_f(E)$ = macroscopic neutron-generation cross-section (cm^{-1})
$\phi(\mathbf{r},E,\mathbf{\Omega})$ = angular flux ($cm^{-2}\cdot s^{-1}$)
$\phi(\mathbf{r},E)$ = scalar flux ($cm^{-2}\cdot s^{-1}$)

The differential scattering term would be expanded using zero and first order Legendre polynomials.

$$\Sigma_s(E\leftarrow E',\mathbf{\Omega}\leftarrow\mathbf{\Omega}') = \frac{1}{2\pi}\Sigma_s(E\leftarrow E',\mu) = \sum_{l=0}^{1}\frac{2l+1}{4\pi}\Sigma_{s,l}(E\leftarrow E')P_l(\mu) \tag{5}$$

where $\mu = \mathbf{\Omega}\cdot\mathbf{\Omega}'$, $P_0(\mu) = 1$ and $P_1(\mu) = \mu$.

Substitute the factorization Eq. (3) into the Eq. (4):

$$[\Sigma(E) + i\mathbf{B}\cdot\mathbf{\Omega}]\varphi(E,\mathbf{\Omega}) = \int_{4\pi} d^2\Omega' \int_0^\infty dE'\Sigma_s(E\leftarrow E',\mathbf{\Omega}\leftarrow\mathbf{\Omega}')\varphi(E',\mathbf{\Omega}') + \frac{\chi(E)}{4\pi K_{eff}}\times\int_0^\infty dE'\nu\Sigma_f(E')\varphi(E') \tag{6}$$

where $\varphi(E)=\int_{4\pi}\varphi(E,\mathbf{\Omega})d^2\Omega$. Substituting Eq. (5) into Eq. (6) and integrating it over the angular domain yields the first equation of the homogeneous leakage model:

$$\Sigma(E)\varphi(E)+iBJ(E)=\int_0^\infty dE'\Sigma_{s0}(E\leftarrow E')\varphi(E')+\frac{\chi(E)}{K_{eff}}\int_0^\infty dE'\nu\Sigma_f(E')\varphi(E') \tag{7}$$

where $J(E)=\frac{1}{B}[\mathbf{B}\cdot\int_{4\pi}d^2\Omega\mathbf{\Omega}\varphi(E,\mathbf{\Omega})]$.

Substitute Eq. (5) into Eq. (6) and integrate with a weighting factor of ω:

$$\varphi(E)=\alpha[B,\Sigma(E)]\left[\int_0^\infty dE'\Sigma_{s0}(E\leftarrow E')\varphi(E')+\frac{\chi(E)}{K_{eff}}\int_0^\infty dE'\nu\Sigma_f(E')\varphi(E')\right]-3i\beta[B,\Sigma(E)]B\int_0^\infty dE'\Sigma_{s1}(E\leftarrow E')J(E')$$

where $\omega=\frac{1}{\Sigma(E)+i\mathbf{B}\cdot\mathbf{\Omega}}$. Substituting Eq. (7) into Eq. (8) yields the second equation of the homogeneous leakage model:

$$\frac{iJ(E)}{B}=\frac{1}{\Sigma(E)\gamma[B,\Sigma(E)]}\left\{\frac{1}{3}\varphi(E)+\int_0^\infty dE'\Sigma_{s1}(E\leftarrow E')\frac{iJ(E')}{B}\right\} \tag{9}$$

where

$$\gamma[B,\Sigma]\cong 1+\frac{4}{15}\left(\frac{B}{\Sigma}\right)^2-\frac{12}{175}\left(\frac{B}{\Sigma}\right)^4+\frac{92}{2625}\left(\frac{B}{\Sigma}\right)^6+o\left(\frac{B}{\Sigma}\right)^8$$

Eq. (7) and Eq. (9) form the homogeneous leakage model. The critical spectrum can be obtained by solving these two equations simultaneously together with a buckling search process. Then the corrected neutron-flux distribution of the single-heterogeneous-assembly transport calculation can be determined for the power-distribution calculation, the cross-section homogenization and so on.

In the homogeneous leakage model, the leakage coefficient and the leakage rate are defined as follows (Hebert, 2009):

$$D(B,E)=\frac{1}{B}\frac{iJ(E)}{\varphi(E)} \tag{10}$$

$$L(E)=D(E,B)B^2\varphi(E) \tag{11}$$

Eq. (11) can be easily condensed over energy groups if the following group-averaged equation is used.

$$L_g=D_g(B)B^2\varphi_g \tag{12}$$

Then the condensation of the leakage coefficient should be carried out as following:

$$D_G=\frac{\sum_{g\in G}D_gB^2\varphi_g}{\sum_{g\in G}B^2\varphi_g} \tag{13}$$

When the homogeneous leakage model is applied in the lattice calculation for pin-cell homogenization, the neutron flux and the current would be corrected by the same corrective factor and the leakage coefficient would be one value for the whole assembly. In order to determine the individual pin-cell diffusion coefficient, the Fick's Law can be utilized.

$$D_i(E)=\frac{1}{3\Sigma_{tr,i}(E)} \tag{14}$$

where $\Sigma_{tr,i}(E)$ = pin-cell macroscopic transport cross-section (cm^{-1})

2.2. Heterogeneous Leakage Model

In the heterogeneous leakage model, the neutron flux is factorized as Eq. (15)

$$\phi(\mathbf{r},E,\mathbf{\Omega})=\varphi(\mathbf{r},E,\mathbf{\Omega})e^{i\mathbf{B}\cdot\mathbf{r}} \tag{15}$$

where all the symbols are the same as Eq. (3) except that the fundamental flux $\varphi(\mathbf{r},E,\mathbf{\Omega})$ is spatially dependent.

The neutron-transport equation for the case of a heterogeneous geometry is shown as Eq. (16):

$$\mathbf{\Omega}\cdot\nabla\phi(\mathbf{r},E,\mathbf{\Omega})+\Sigma(r,E)\phi(\mathbf{r},E,\mathbf{\Omega})=\int_{4\pi}d^2\Omega'\int_0^\infty dE'\Sigma_s(r,E\leftarrow E',\mathbf{\Omega}\leftarrow\mathbf{\Omega}')\phi(\mathbf{r},E',\mathbf{\Omega}')+\frac{\chi(E)}{4\pi K_{eff}}\int_0^\infty dE'\nu\Sigma_f(r,E')\phi(\mathbf{r},E') \tag{16}$$

where all the symbols are the same as Eq. (4) except their dependence of spatial variable.

Substitute the factorization into the neutron-transport equation:

$$\Omega\cdot\nabla\varphi(\mathbf{r},E,\Omega)+\Omega\cdot\varphi(\mathbf{r},E,\Omega)\nabla(i\mathbf{B}\cdot\mathbf{r})+\Sigma(\mathbf{r},E)\varphi(\mathbf{r},E,\Omega)=\int_{4\pi}d^2\Omega'\int_0^\infty dE'\Sigma_s(\mathbf{r},E\leftarrow E',\Omega\leftarrow\Omega')\varphi(\mathbf{r},E',\Omega')+\frac{\chi(\mathbf{r},E)}{4\pi K_{eff}}\int_0^\infty dE'\nu(\mathbf{r},E')\Sigma_f(\mathbf{r},E')\varphi(\mathbf{r},E') \tag{17}$$

where $\varphi(\mathbf{r},E)=\int_{4\pi}\varphi(\mathbf{r},E,\Omega')d^2\Omega'$

Substituting Eq. (5) into Eq. (17) leads to the following equation:

$$\Omega\cdot\nabla\varphi(\mathbf{r},E,\Omega)+\Sigma(\mathbf{r},E)\varphi(\mathbf{r},E,\Omega)=\frac{1}{4\pi}Q(\mathbf{r},E,\Omega)-i\mathbf{B}\Omega\cdot\varphi(\mathbf{r},E,\Omega) \tag{18}$$

where

$$Q(\mathbf{r},E,\Omega)=\int_0^\infty \mathrm{d}E'\Sigma_{s0}(\mathbf{r},E\leftarrow E')\varphi(\mathbf{r},E')+\frac{\chi(\mathbf{r},E)}{K_{eff}}\int_0^\infty \mathrm{d}E'\nu(\mathbf{r},E')\Sigma_f(\mathbf{r},E')\varphi(\mathbf{r},E')+\int_{4\pi}\mathrm{d}^2\Omega'\int_0^\infty \mathrm{d}E'3\Sigma_{s1}(\mathbf{r},E\leftarrow E')\mu\varphi(\mathbf{r},E',\Omega') \tag{19}$$

Smearing the source of Eq. (18) within the angular domain yields the first equation of the heterogeneous leakage model:

$$\Omega\cdot\nabla\varphi(\mathbf{r},E,\Omega)+\Sigma(\mathbf{r},E)\varphi(\mathbf{r},E,\Omega)=\frac{1}{4\pi}[Q(\mathbf{r},E)-iB\varphi_1(\mathbf{r},E)] \tag{20}$$

where

$$Q(\mathbf{r},E)=\int_0^\infty \mathrm{d}E'\Sigma_{s0}(\mathbf{r},E\leftarrow E')\varphi(\mathbf{r},E')+\frac{\chi(\mathbf{r},E)}{K_{eff}}\int_0^\infty \mathrm{d}E'\nu(\mathbf{r},E')\Sigma_f(\mathbf{r},E')\varphi(\mathbf{r},E')$$

$$iB\varphi_1(\mathbf{r},E)=\int_{4\pi}i\mathbf{B}\Omega\cdot\varphi(\mathbf{r},E,\Omega)\mathrm{d}\Omega$$

The weighting factor showed in Eq. (23) is used to integrate Eq. (19) over the angular domain, yielding Eq. (24) as the second equations of the heterogeneous model (Grimstone et al., 1990):

$$\omega(\mathbf{r},\Omega)=\frac{1}{\Sigma(\mathbf{r},E)+i\mathbf{B}\Omega} \tag{21}$$

$$\mathbf{\Omega}\cdot\nabla\varphi_1(\mathbf{r},E,\mathbf{\Omega})+\Sigma(\mathbf{r},E)\varphi_1(\mathbf{r},E,\mathbf{\Omega})=\frac{1}{4\pi\gamma[B,\bar{\Sigma}(E)]}\left[\frac{1}{3}\varphi_0(\mathbf{r},E)B^2+\int_0^\infty \mathrm{d}E'\Sigma_{s1}(\mathbf{r},E\leftarrow E')\varphi_1(\mathbf{r},E')\right] \tag{22}$$

The critical spectrum of each pin cell can be obtained by solving Eq. (20) and Eq. (22) simultaneously together with a buckling search process. The corrected neutron-flux distribution of the single heterogeneous assembly transport calculation can be determined after the buckling search process. This model can provide space-dependent leakage coefficient (LC) Benoist et al., 1994; Hebert, 2009:

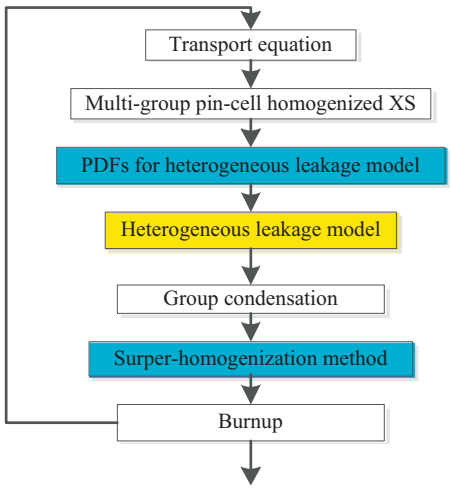


Fig. 1. Calculation flow of heterogeneous leakage model.

$$D_i(B,E) = \frac{1}{B}\frac{iJ_i(E)}{\varphi_i(E)} \tag{23}$$

$$L_i(E) = D_i(E,B)B^2\varphi_i(E) \tag{24}$$

2.3. Cooperation of heterogeneous leakage model and homogenization

In the heterogeneous leakage model for pin-cell homogenization, the pin-cell discontinuity factors (Zhang et al., 2016, 2016) (PDF) should be determined before performing the buckling search. Because the PDFs can preserve the pin-cell-homogenized problem unchanged compared with the original assembly problem. For example, when a critical buckling search is performed for a single-assembly problem whose k_{eff} is equal to 1.0, the global spectrum should be equal to the infinite spectrum. However, without PDFs, the global spectrum determined by the heterogeneous leakage cannot be equal to the infinite one. So the heterogeneous leakage model must cooperate with the pin-cell-homogenized cross-section together with the PDF. In this paper, the discrete ordinate method (Zhitao et al., 2014) is used to solve the equations of the heterogeneous leakage. The corresponding PDF would be calculated for the solver.

After a buckling search, the homogenization method should be super-homogenization method (Zhang et al., 2016, 2016; Hebert and Mathonniere, 1993) rather than GET. This is because that the current on each interface is affected by two different global spectrums of the two adjacent pin cells. It is in a dilemma to correct one neutron current by two global spectrums. The calculation flow is shown in Fig. 1.

2.4. Buckling search

Considering the fact that the buckling appears to be the eigenvalue of leakage model equation, the legacy power method can be employed, named as the power-method scheme. Meanwhile, the buckling can also be taken as a kind of pseudo boron, providing a linear-interpolation scheme as the second option (Li et al., 2010). In addition, a rapid search scheme is also proposed as the third option based on the neutron balance.

2.4.1. The power method scheme

If the buckling for the n'th iteration is denoted as $B^2(n)$, the initial guess is therefore $B^2(1)$. For the $(n+1)$'th iteration, the new buckling can be calculated as following:

$$B^2(n+1) = B^2(n) + \Delta B^2(n) \tag{25}$$

where $\Delta B^2(n)$ can be calculated by the linear interpolation between $1/k_{\text{eff}}$ and B^2.

$$\Delta B^2(n) = A(n)\left(\frac{1}{k_{eff}^{req}} - \frac{1}{k_{eff}(n)}\right) \tag{26}$$

where k_{eff}^{req} is the targeted k_{eff} and $A(n)$ is the estimated slope of B^2 in terms of $1/k_{\text{eff}}$. At the end of the first iteration, this slope can be estimated by using the following formula:

$$A(1) = \frac{V\phi(1)D(1)}{k_{eff}(1)} \tag{27}$$

where $V = \sum_i V_i$, $\phi(1) = \sum_g\sum_i \frac{V_i\phi_{i,g}(1)}{V_i}$, $D(1) = \frac{V\phi(1)}{3\sum_g\sum_i V_i\phi_{i,g}(1)\Sigma_{tr,i,g}(1)}$ is an approximated value at this stage.

2.4.2. The linear interpolation scheme

Considering the fact that linear interpolation is usually employed for the critical boron concentration (CBC) search in the PWR core analysis, it can also be employed for the buckling search as:

$$B^2(n+1) = B^2(n-1) + \frac{k_{eff}^{req} - k_{eff}(n-1)}{k_{eff}(n) - k_{eff}(n-1)}[B^2(n) - B^2(n-1)] \tag{28}$$

Compared the Eq. (25) and Eq. (28), the difference mainly lies in the term of $\Delta B^2(n)$. Rewrite Eq. (28) into the following form:

$$B^2(n+1) = B^2(n) + \left(\frac{1}{k_{eff}^{req}} - \frac{1}{k_{eff}(n)}\right)\frac{[B^2(n) - B^2(n-1)]}{\frac{1}{k_{eff}(n)} - \frac{1}{k_{eff}(n-1)}} \times \frac{k_{eff}^{req}}{k_{eff}(n-1)} \tag{29}$$

which can be further presented into the following form:

$$B^2(n+1) = B^2(n) + \frac{k_{eff}^{req}}{k_{eff}(n-1)}A(n)\left(\frac{1}{k_{eff}^{req}} - \frac{1}{k_{eff}(n)}\right) \tag{30}$$

It can be found that a relaxation parameter is utilized in this scheme compared with the power method scheme.

2.5.3. The neutron balance scheme

It is unnecessary to care about the computational cost for the homogenized problem in the homogeneous leakage model. For the heterogeneous leakage model, however, the computational cost is considerable. In order to minimize the computational costs of the buckling search, a scheme for rapid convergence to update the buckling is proposed based on neutron balance.

The heterogeneous leakage equations can be obtained as follows after a multi-group discretization at the n'th iteration:

$$\begin{aligned}&\boldsymbol{\Omega}\cdot\nabla\varphi_{0,g}^n(\mathbf{r},\boldsymbol{\Omega}) + \Sigma_g(\mathbf{r})\varphi_{0,g}^n(\mathbf{r},\boldsymbol{\Omega})\\ &= \frac{1}{4\pi}\left[Q_{s0,g}^n(\mathbf{r}) + \frac{1}{k_{eff}(n)}Q_{f,g}^n(\mathbf{r}) - \varphi_{1,g}^{n+1}(\mathbf{r})\right]\end{aligned} \tag{31}$$

$$\begin{aligned}&\boldsymbol{\Omega}\cdot\nabla\varphi_{1,g}^n(\mathbf{r},\boldsymbol{\Omega}) + \Sigma_g(\mathbf{r})\varphi_{1,g}^n(\mathbf{r},\boldsymbol{\Omega})\\ &= \frac{1}{4\pi\gamma_g(B)}\left[\frac{1}{3}\varphi_{0,g}^n(\mathbf{r})B^2(n) + Q_{s1,g}^n(\mathbf{r})\right]\end{aligned} \tag{32}$$

where all the symbols are the same as Eq. (20) and Eq. (22). Integrate Eq. (32) over the angular domain and then substitute it into Eq. (31), we can get the following equation:

Table 2
Iterative procedure of the homogeneous problem.

Iteration	Homogeneous Leakage Model		Heterogeneous Leakage Model	
	k_{eff}	Buckling	k_{eff}	Buckling
1	1.14623	0.0000E+00	1.14623	0.0000E+00
2	1.14617	1.0000E−06	1.14617	1.0000E−06
3	0.99748	2.7414E−03	0.99747	2.7414E−03
4	1.00005	2.6881E−03	1.00005	2.6881E−03
5	1.00000	2.6892E−03	1.00000	2.6892E−03

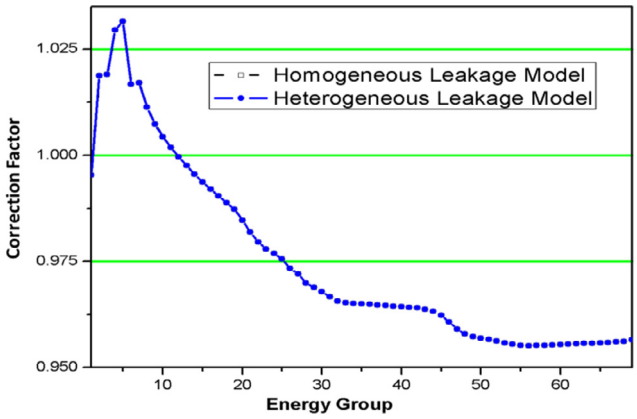


Fig. 2. 69-Group flux-spectrum correction factor for the homogeneous problem.

$$\boldsymbol{\Omega}\cdot\nabla\varphi^{n}_{0,g}(\mathbf{r},\boldsymbol{\Omega})+\Sigma_g(\mathbf{r})\varphi^{n}_{0,g}(\mathbf{r},\boldsymbol{\Omega})=\left\{\frac{1}{4\pi}\left[Q^{n}_{s0,g}(\mathbf{r})+\frac{1}{k^{n}_{eff}}Q^{n}_{f,g}(\mathbf{r})-\frac{1}{\Sigma_g(\mathbf{r})}\frac{1}{\gamma_g(B)}\left[\frac{1}{3}\varphi^{n}_{0,g}(\mathbf{r})B^2(n)+Q^{n}_{s1,g}(\mathbf{r})\right]-\int_{\Omega}\boldsymbol{\Omega}\cdot\nabla\varphi^{n}_{1,g}(\mathbf{r},\boldsymbol{\Omega})d\Omega\right]\right\} \tag{33}$$

For the targeted k_{eff}, theoretically, there exists a similar equation:

$$\boldsymbol{\Omega}\cdot\nabla\varphi^{req}_{0,g}(\mathbf{r},\boldsymbol{\Omega})+\Sigma_g(\mathbf{r})\varphi^{req}_{0,g}(\mathbf{r},\boldsymbol{\Omega})=\left\{\frac{1}{4\pi}\left[Q^{req}_{s0,g}(\mathbf{r})+\frac{1}{k^{req}_{eff}}Q^{req}_{f,g}(\mathbf{r})-\frac{1}{\Sigma_g(\mathbf{r})}\frac{1}{\gamma^{req}_g(B)}\left[\frac{1}{3}\varphi^{req}_{0,g}(\mathbf{r})B^2(n)+Q^{req}_{s1,g}(\mathbf{r})\right]-\int_{\Omega}\boldsymbol{\Omega}\cdot\nabla\varphi^{req}_{1,g}(\mathbf{r},\boldsymbol{\Omega})d\Omega\right]\right\} \tag{34}$$

With the assumption that the n'th iteration and the converged iteration share the same neutron flux distribution and the parameter $\gamma_g(B)$, a new buckling update formula can be obtained:

$$B^2(req)=B^2(n)+\left(\frac{1}{k^{req}_{eff}}-\frac{1}{k_{eff}(n)}\right)\frac{\sum_g\int_V Q^{n}_{f,g}(\mathbf{r})dV}{\sum_g\int_V\frac{1}{3\Sigma_g(\mathbf{r})\gamma^{n}_g(B)}\varphi^{n}_{0,g}(\mathbf{r})dV} \tag{35}$$

3. Numerical results

Both the homogeneous and heterogeneous leakage models are implemented into our in-house developed PWR lattice code Bamboo-Lattice (Li et al., 2015; Chen et al., 2008; He et al., 2014; Huang et al., 2016), which employs a two-dimensional modular MOC transport solver. Three test problems are presented in this section. Firstly, a single-homogeneous-assembly calculation followed by full-assembly homogenization was employed to show the equivalence between the homogeneous and heterogeneous leakage models in the special case. Secondly, several single-heterogeneous-assembly calculations followed by pin-cell homogenization cases were carried out to show the differences between the homogeneous and heterogeneous leakage models. Finally, a 2D PWR core pin-by-pin calculation was performed to assess the performances of the leakage models.

3.1. Single-assembly problem with full-assembly homogenization

Theoretically, the heterogeneous leakage model would be exactly the same as the homogeneous one for a single-homogeneous-assembly calculation. For a 2D homogeneous problem, a 69-group (WIMS D4 format) transport calculation was car-

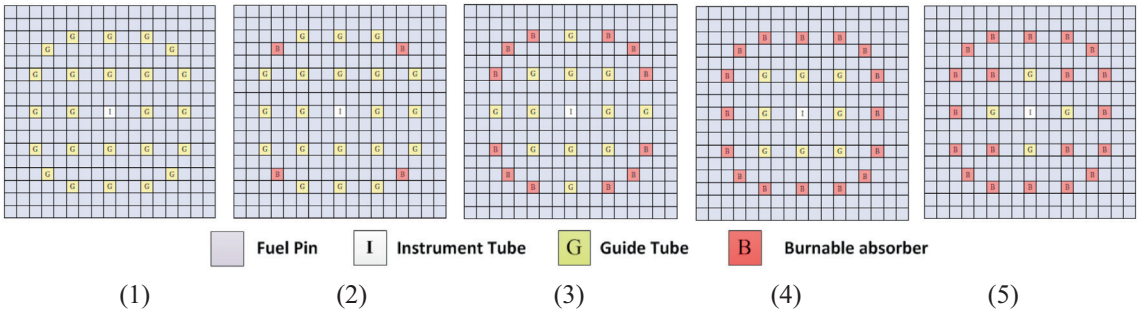


Fig. 3. Five geometries of assemblies.

Table 3
Models of cross-section generation.

Fuel Materials	UO_2 1.60 w/o UO_2 2.40 w/o UO_2 3.10 w/o	Single-cell calculation
Other Materials	Burnable absorber Clad/Guide/Coolant	3.10% w/o assembly calculation under the 2th configuration in Fig. 3
Reflector	Baffle/Reflector	Two-assembly calculation

Table 4
Flux-spectrum correction factor for Single-assembly problems.

CASES		k_{eff}	Flux-spectrum correction factor							
			Group	1	2	3	4	5	6	7
1	1.60%	1.00166	Hom	1.0005	1.0003	1.0000	0.9999	0.9998	0.9998	0.9998
			Het	1.0005	1.0003	1.0000	0.9999	0.9997	0.9997	0.9997
2	2.40%	1.12600	Hom	1.0388	1.0181	0.9998	0.9922	0.9841	0.9834	0.9836
			Het	1.0388	1.0181	0.9998	0.9922	0.9841	0.9834	0.9836
3	3.10%	1.18264	Hom	1.0552	1.0249	0.9988	0.9881	0.9782	0.9772	0.9775
			Het	1.0552	1.0250	0.9987	0.9881	0.9782	0.9773	0.9775
4	2.40% 12BA	1.00267	Hom	1.0008	1.0004	1.0000	0.9998	0.9997	0.9997	0.9997
			Het	1.0008	1.0004	1.0000	0.9998	0.9997	0.9996	0.9996
5	2.40% 16BA	0.96448	Hom	0.9888	0.9949	1.0003	1.0024	1.0044	1.0046	1.0046
			Het	0.9888	0.9949	1.0003	1.0024	1.0044	1.0046	1.0045
6	3.10% 4BA	1.14167	Hom	1.0430	1.0193	0.9989	0.9906	0.9831	0.9824	0.9826
			Het	1.0430	1.0194	0.9989	0.9906	0.9831	0.9824	0.9826
7	3.10% 16BA	1.03034	Hom	1.0094	1.0041	0.9996	0.9979	0.9964	0.9963	0.9963
			Het	1.0094	1.0041	0.9997	0.9979	0.9964	0.9962	0.9963
8	3.10% 20BA	0.99554	Hom	0.9986	0.9994	1.0001	1.0003	1.0005	1.0005	1.0005
			Het	0.9986	0.9994	1.0001	1.0003	1.0005	1.0005	1.0005

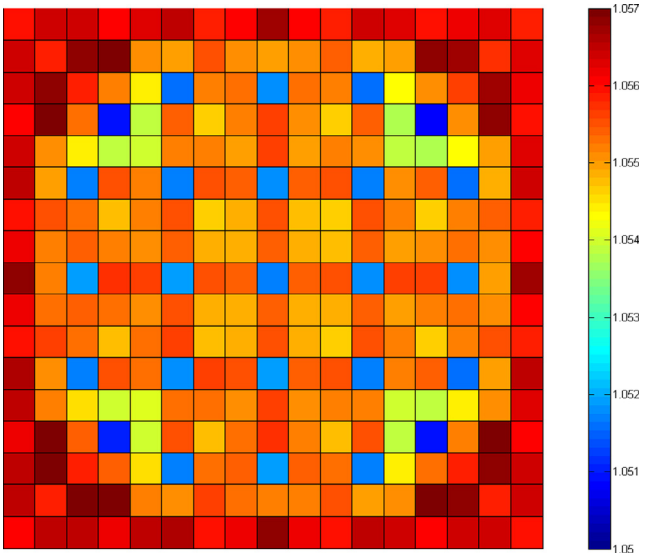


Fig. 4. First-group flux-spectrum correction factors of each pin cell for CASE 3.

ried out with either 69-group homogeneous leakage model or heterogeneous leakage model. The iterative procedure and the 69-group flux-spectrum correction factors are respectively shown in Table 2 and Fig. 2. There is no difference on the correction factors between the homogeneous leakage model and the heterogeneous leakage model. The iterative procedures are almost exactly the same as expected.

3.2. Single-assembly problems with pin-cell homogenization

In order to analyze the two leakage models, 8 single-assembly tests consisting of three enrichments (1.60%, 2.40% and 3.1%) and five burnable absorber loadings as in Fig. 3 were calculated and homogenized at pin-cell level. The 7-group heterogeneous cross-sections are obtained by pre-evaluating the cases in Table. 3 using the Bamboo-Lattice code.

The flux-spectrum correction factor of each group from the homogeneous leakage model and the volume-averaged correction factor of the whole assembly from the heterogeneous leakage model are shown in Table 4. It can be found that they are almost the same and the maximum difference is less than 0.1%. The correction factor will be harder than the local spectrum when k_{eff} is larger than 1.0, while it is opposite when k_{eff} is smaller than 1.0.

The first-group flux-spectrum correction factors of each pin cell for case 3 are shown in Fig. 4. It can be found that the correction

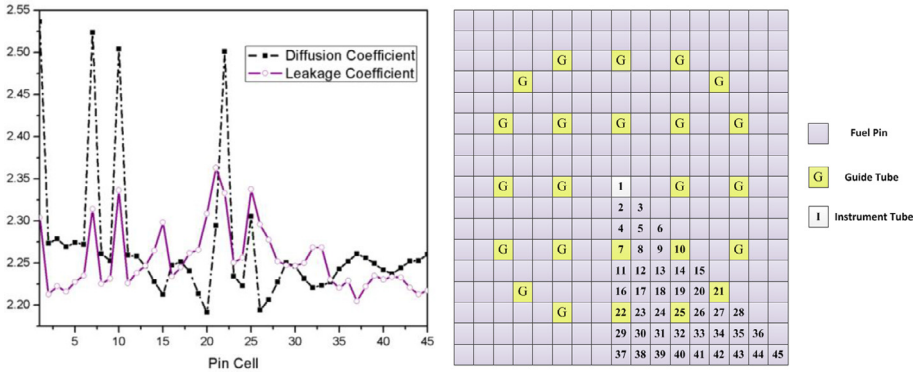
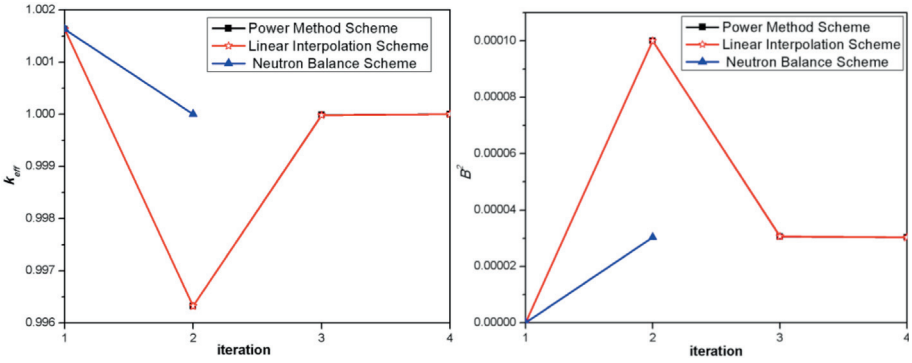
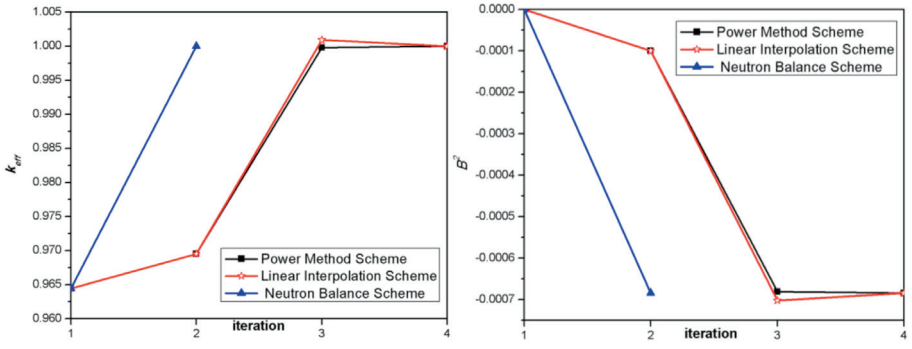


Fig. 5. First-group Leakage Coefficients and Diffusion Coefficients.



a) k_{eff} of each iteration step b) B^2 of each iteration step

Fig. 6. Iteration Procedure of CASE 1.



a) k_{eff} of each iteration step b) B^2 of each iteration step

Fig. 7. Iteration Procedure of CASE 5.

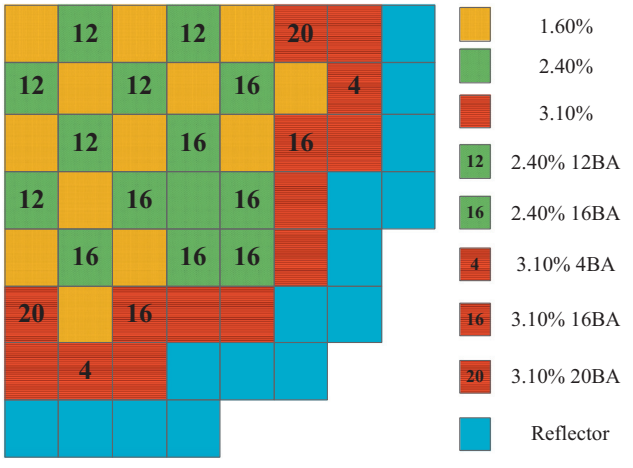


Fig. 8. Configuration of the 1/4 PWR Core.

factors of the guide tube or burnable absorber are different from that of fuel pins. The homogeneous leakage model cannot represent the differences of the correction factors between different pins. What's more, for the pin-cell homogenization, the homogeneous leakage model provides only one leakage coefficient for the entire assembly consisting of 289 pins. The heterogeneous leakage model can provide separated leakage coefficient for each pin. The first-group pin-cell leakage coefficients and diffusion coefficients in case 3 are shown in Fig. 5. There is a large difference existed between them, it would be further analyzed that which one is more accurate for the whole core calculation in the next section.

The performances of the three different methods to search the targeted buckling are also compared with the initial values of B^2 fixed as 0. The iteration procedure of the buckling search of case 1 about k_{eff} and B^2 is shown in Fig. 6 and that of CASE 5 is shown in Fig. 7. It can be found that whether k_{eff} is larger or smaller than 1.0, the computational cost of the power-method scheme and that

Table 5
The results of the 2D whole core problem.

Leakage Model	Type of Coefficient	Energy Groups	k_{eff}	k_{eff} Error (pcm)	Pin-Power RMS Error % (Max Error)
W/O	DC	7	1.00001	1	1.01(4.35)
Hom			1.00001	1	1.01(4.34)
Het			1.00001	1	1.01(4.31)
Het	LC		1.00029	29	0.87(4.02)
W/O	DC	2	1.00066	66	1.92(4.13)
Hom			0.99979	-21	1.36(3.86)
Het			0.99979	-20	1.35(3.79)
Het	LC		1.00010	10	0.64(3.54)

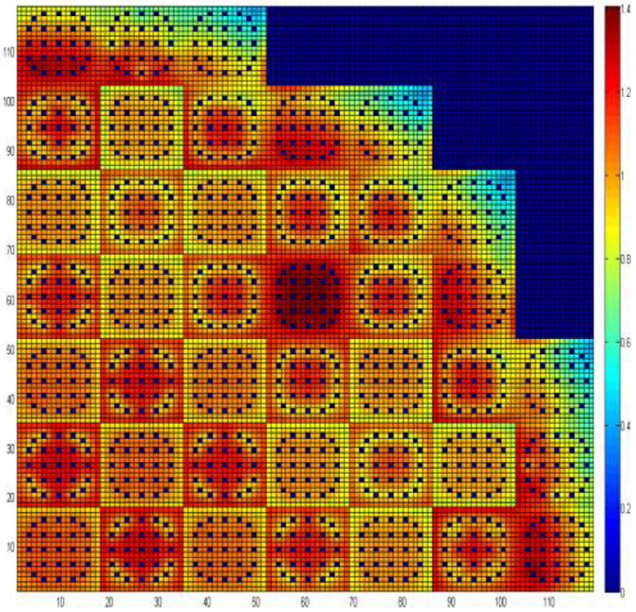


Fig. 9. The reference pin-power distribution.

of the linear-interpolation scheme are almost the same, requiring about four iterations to converge. For the neutron balance scheme, in contrast, usually two iterations are enough.

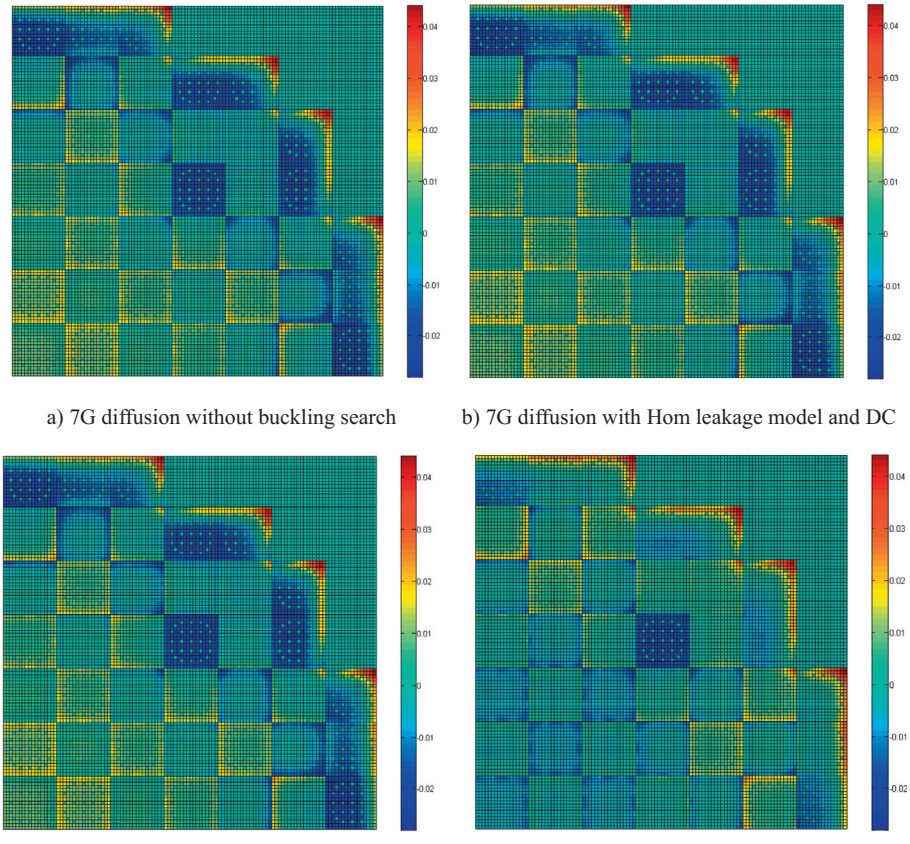
3.3. Whole core problem with pin-cell homogenization

The core showed in Fig. 8 consists of eight kinds of assemblies mentioned in the former section.

Several schemes were carried out to test the performances of the leakage models:

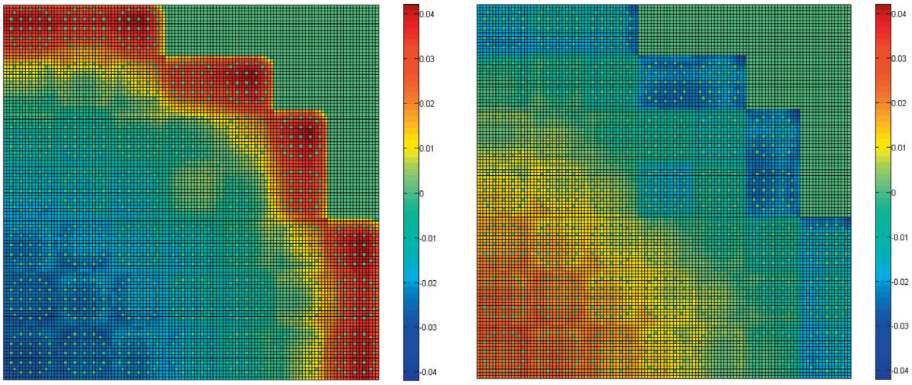
(1) The reference solution was provided by a 2D whole-core one-step transport calculation using 7-group heterogeneous cross-section obtained from Section 3.2.
(2) Single-assembly calculations with reflective boundary conditions without leakage model was performed first to provide the pin-cell homogenized 2-/7-group cross-sections, followed by the pin-by-pin core-diffusion calculations (Li et al., 2013; Yunzhao et al., 2014; Yang et al., 2016; Cao et al., 2013).
(3) Single-assembly calculations with reflective boundary conditions with 7-group homogeneous/heterogeneous leakage model was performed first to provide the pin-cell-homogenized 2-/7-group parameters, followed by the pin-by-pin core-diffusion calculations. The diffusion coefficient (DC) is used in the diffusion calculation for the homogeneous leakage model, while either diffusion coefficient or space-dependent leakage coefficient (LC) is used in the diffusion calculation for the heterogeneous leakage model.

Table 5 represents the summary of results and the reference pin-power distribution is showed in Fig. 9. The pin-power relative error distributions of 7- and 2-group diffusion pin-by-pin calculations are shown in Fig. 10 and Fig. 11 respectively. It can be found

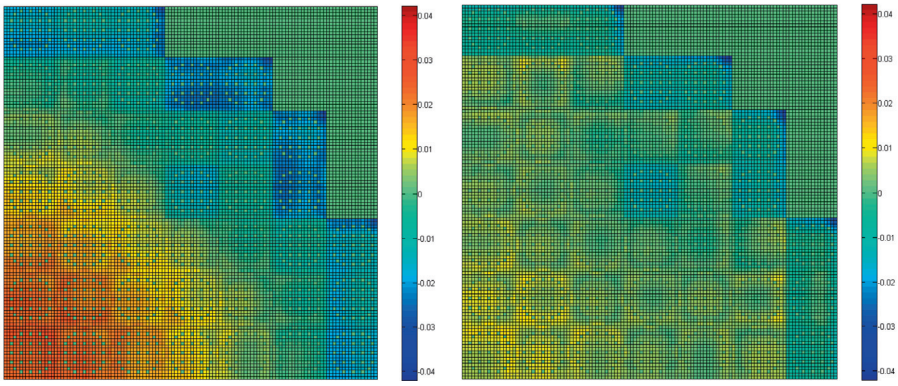


a) 7G diffusion without buckling search
b) 7G diffusion with Hom leakage model and DC
c) 7G diffusion with Het leakage model and DC
d) 7G diffusion with Hom leakage model and LC

Fig. 10. Relative pin-power error of 7G diffusion pin-by-pin calculation.



a) 2G diffusion without buckling search b) 2G diffusion with Hom leakage model and DC



c) 2G diffusion with Het leakage model and DC d) 2G diffusion with Hom leakage model and LC

Fig. 11. Relative pin-power error of 2G diffusion pin-by-pin calculation.

that both of the two leakage models can improve the accuracy of the pin-by-pin core-diffusion calculations. Almost the same results are observed for the two leakage models when the diffusion coefficient is determined by the transport cross-section. The pin-by-pin calculations with the space-dependent leakage coefficient obtained from the heterogeneous leakage model show the most accurate results.

4. Conclusions

For the pin-by-pin two-step scheme, a leakage model is required in the lattice calculation because of the reflective boundary condition. The derivation of the formula of the leakage model is introduced, and the implementations of the homogeneous and heterogeneous leakage models are described. The homogeneous leakage model applied in pin-cell homogenization will lead to the same corrective factor to correct the neutron flux and the current, while the diffusion coefficient based on Fick's Law would be utilized in the core calculation. When the heterogeneous leakage model is applied to pin-cell homogenization, before buckling search, pin-cell discontinuity factor must be generated for the pin-cell homogenized assembly. After buckling search and spectrum leakage modification, the homogenization method should be super-homogenization method rather than GET due to the different critical spectrums of adjacent pin cells.

A rapid buckling search scheme is proposed and three different schemes were compared with each other on single-assembly problems. It can be found that the computational cost of the power-method scheme and that of the linear-interpolation scheme according to CBC are almost the same. Their costs are almost twice than the newly proposed neutron balance scheme.

By looking at the relative error distributions, it can be found that the homogeneous leakage model works effectively for the pin-cell homogenization, while the heterogeneous leakage model with the space-dependent leakage diffusion provides better accuracy. The leakage model can only take the leakage into consideration approximately. The environment effect aroused by the reflective boundary condition needs more investigation and improvements.

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