Group Constants Generation Based on NECP-MCX Monte Carlo Code

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Abstract. The reliability of few-group constants generated by lattice physics calculation is significant for the accuracy of the conventional two-step method in neutronics calculation. The deterministic method is preferred in the lattice calculation due to its efficiency. However, it is difficult for the deterministic method to treat the resonance self-shielding effect accurately and handle complex geometries. Compared to the deterministic method, the Monte Carlo method has the characteristics of using continuous-energy cross section and the powerful capability of geometric modeling. Therefore, the Monte Carlo particle transport code NECP-MCX is extended in this study to generate assembly-homogenized few-group constants. The cumulative migration method is adopted to generate the accurate diffusion coefficient and the leakage correction is performed using the homogeneous fundamental mode approximation. For the verification of the generated few-group constants, a code sequence named MCX-SPARK is built based on NECP-MCX and a core analysis code SPARK to perform the two-step calculation. The physics start-up test of the HPR1000 reactor is simulated using the MCX-SPARK sequence. The results from MCX-SPARK agree well with the results from the design report and a deterministic two-step code Bamboo-C. It is concluded that the NECP-MCX has the ability to generate accurate few-group constants.

Keywords: Few-group constant · Monte Carlo · Two-step · NECP-MCX · HPR1000

1 Introduction

The two-step method [1] is the most popular approach for the practical application of neutronics calculations. During the two-step calculation, a series of lattice physics calculations are performed to evaluate the spatial and spectral flux of fuel assemblies under different state-points, and these fluxes are homogenized and collapsed to generate the assembly-homogenized few-group constants. These few-group constants are then parameterized and inputted into the nodal diffusion code to obtain the interested quantities for reactor design or analysis. Conventionally, the deterministic method like the collision probability method [1] or the method of characteristics [2] is preferred in the stage of lattice physics calculation since its efficiency, and many applications have

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proven its validity. However, two main drawbacks still exist in the deterministic lattice physics codes in spite of their success, which will limit their further application. The first drawback is that the resonance self-shielding calculation like the subgroup calculation [3] must be performed to evaluate a set of problem-dependent cross-sections before the transport calculation. Some modifications or extensions must be added to the conventional resonance self-shielding methods and adopted in a deterministic lattice physics code to obtain accurate self-shielded cross-sections. And these treatments are only specific to their target problem. The second drawback is that the range of a deterministic lattice physics code for geometric modeling is limited, and the problem with complicated geometry is often replaced by an approximated model in a deterministic lattice physics model.

In order to overcome the drawbacks in the deterministic lattice physics calculation, the Monte Carlo (MC) method for the generation of the few-group constants has drawn some attention [4–7]. MC is an approach that tracks a large number of neutrons in a stochastic way and obtains the interested quantities by calculating the expected value from repeated tallies. Compared to the deterministic method, the neutron is tracked under the detailed geometric model and continuous-energy cross-section information. In addition, the neutron under MC tracking is simulated through real physical details if it interacts with a nuclide. These characteristics of the MC method make it a more rigorous and generalized method than the deterministic method. The main drawback of the MC method is that its calculation efficiency is far below the deterministic method, but the MC method is suitable to be calculated in parallel, and the improvement of the parallel computational technique and super-computer permit the MC method to be a more efficient method.

In this paper, we extend the MC code NECP-MCX [8] to generate assembly-homogenized few-group constants, and the physical start-up test of HPR1000 [9] is simulated for verification. The detailed methodology is introduced in Sect. 2, the method for verification and the numerical results are given in Sect. 3, and Sect. 4 gives the conclusion and discussion.

2 Methodology

2.1 Homogenization Method

During homogenization, three important physical quantities including the integrated reaction rates, the integrated net current, and the eigenvalue must be conserved for the homogenized assembly [10]. The equations below represent these conservation conditions in sequence:

$$\int_V \Sigma_{x,g}^{\text{hom}} \phi_g^{\text{hom}}(\vec{r}) d\vec{r} = \int_{E_g}^{E_{g-1}} \int_V \Sigma_x^{\text{het}}(\vec{r}, E) \phi^{\text{het}}(\vec{r}, E) d\vec{r} dE \tag{1}$$

where $\Sigma_{x,g}$ represents the cross-section for reaction type x and group g, ϕ is the scalar flux. The superscript "hom" and "het" represents the homogenized and heterogeneous assembly, respectively.

$$-\int_{S_k} D_g^{\text{hom}} \nabla \phi_g^{\text{hom}}(\vec{r}) ds = \int_{E_g}^{E_{g-1}} \int_{S_k} J^{\text{het}}(\vec{r}, E) ds dE \tag{2}$$

where k represents the k-th surface of assembly, J is the net-current, and D_g is the diffusion coefficient.

$$\begin{aligned} &-\sum_{k=1}^{K}\int_{S_k} D_g^{\text{hom}}\nabla\phi_g^{\text{hom}}(\vec{r})ds+\int_V \Sigma_{t,g}^{\text{hom}}\phi_g^{\text{hom}}(\vec{r})d\vec{r} \\ &=\sum_{g'=1}^{G}\int_V \Sigma_{s,g'\to g}^{\text{hom}}\phi_{g'}^{\text{hom}}(\vec{r})d\vec{r} \\ &+\frac{1}{k_{eff}^{\text{het}}}\sum_{g'=1}^{G}\int_V \chi_g^{\text{hom}}\nu\Sigma_{f,g'}^{\text{hom}}\phi_{g'}^{\text{hom}}(\vec{r})d\vec{r} \end{aligned} \tag{3}$$

where k_{eff}^{het} is the eigenvalue before homogenization. Equation (3) is conserved if the first two conditions are satisfied.

It is impractical to perform the homogenization based on the above equation strictly, therefore, in the conventional homogenization process, the heterogeneous assembly flux is approximated by the lattice physics calculation of a 2D assembly with zero net current, then the homogenized cross-sections are be calculated as:

$$\Sigma_{x,g}^{\text{hom}}=\frac{\int_{E_g}^{E_{g-1}}\int_V \Sigma_x^A(\vec{r},E)\phi^A(\vec{r},E)d\vec{r}dE}{\int_{E_g}^{E_{g-1}}\int_V \phi^A(\vec{r},E)d\vec{r}dE} \tag{4}$$

where the superscript A represents the assembly with net zero current.

The diffusion coefficient is approximated by:

$$D_g^{\text{hom}}=\frac{\int_{E_g}^{E_{g-1}}\int_V D(\vec{r},E)\phi^A(\vec{r},E)d\vec{r}dE}{\int_{E_g}^{E_{g-1}}\int_V \phi^A(\vec{r},E)d\vec{r}dE} \tag{5}$$

Equations (4) and (5) cannot guarantee the conservations described before, therefore, an additional set of quantities, called the assembly discontinuous factors (ADFs) [10], are calculated and delivered to the downstream nodal diffusion code to conserve the integrated reaction rates and net currents. The ADFs are defined as:

$$f_{g,k}=\frac{\phi_{g,k}^{\text{het}}}{\phi_{g,k}^{\text{hom}}} \tag{6}$$

where $f_{g,k}$ is the ADF in the group g and k-th surface. $\phi_{g,k}^{\text{het}}$ and $\phi_{g,k}^{\text{hom}}$ are the surface flux of the assembly in the heterogeneous and homogeneous condition, respectively.

In addition, the assembly with zero net current differs from the assembly in a critical core, therefore, the leakage correction process is adopted by deterministic lattice physics code to evaluate the critical spectrum under its multigroup structure. This spectrum is then used to collapse multigroup cross-sections. In order to make this approach embedded in the MC homogenization, the original tally during MC simulation is based on a multigroup structure to calculate a critical spectrum for further treatments.

As described before, the basic process for MC homogenization in NECP-MCX follows:

a) MC reaction rate tallies with appropriate estimators (analog estimator for scattering matrix and fission spectrum, track-length estimator for others) are performed in the multigroup structure;
b) Flux-volume weighting are performed to calculate the multigroup cross-section. Then the leakage correction is performed based on the multigroup cross-sections to obtain a critical spectrum;
c) The critical spectrum from b) is used to calculate final few-group constants;
d) Evaluate the ADFs.

Some details must be determined from the procedures above: The tally of the diffusion coefficient in MC code, the methodology for leakage correction, and the calculation of ADFs. And these details are described below.

2.2 Generation of Diffusion Coefficient

Derived from P1 equation and Fick's law, the diffusion coefficient can be defined as:

$$D(\vec{r}, E) = \frac{1}{3\left[\Sigma_t(\vec{r}, E) - \frac{\int_0^\infty dE' \Sigma_{s,1}(\vec{r}, E' \to E) J(\vec{r}, E')}{J(\vec{r}, E)}\right]} \tag{7}$$

where $\Sigma_{s,1}$ denotes the 1-order scattering matrix, and $J(\vec{r}, E)$ is the magnitude of current at $\vec{r}$.

However, it is impractical to tally the volume-integrated current from MC calculation since the cancellation of neutron tracks at different directions will lead to an unacceptable statistic error. Therefore, a cumulative migration method [11] is adopted in this study to generate the diffusion coefficient.

In the one-group diffusion theory, the migration area is defined as [12]:

$$M^2 = \frac{D}{\Sigma_a} = \frac{1}{6}\overline{r_m^2} \tag{8}$$

where M^2 is the migration area, D is the diffusion coefficient, Σ_a is the absorption cross-section, and $\overline{r_m^2}$ is the average square flight length of a neutron that starts from its born site to the absorbed site.

The multigroup extension for the Eq. (8) can be realized by replacing the one-group absorption cross-section with the multigroup removal cross-section:

$$M_g^2 = \frac{D_g}{\Sigma_{r,g}} = \frac{1}{6}\overline{r_{m,g}^2} \tag{9}$$

According to Eq. (9), the calculation of diffusion coefficient is given as follows:

a) During MC calculation, tally the $\overline{r_{m,g}^2}$, and notates its raw summation as T_g;
b) The multigroup migration area M_g^2 is calculated by averaging T_g by removal reaction rate;

c) The multigroup diffusion coefficient is finally calculated by:

$$D_g = M_g^2 \Sigma_{r,g} = \frac{T_g}{\Sigma_{r,g}\phi_g} \Sigma_{r,g} = \frac{T_g}{\phi_g} \tag{10}$$

However, the application of cumulative migration method is limited with infinite problems like assemblies with reflective boundaries. Therefore, an alternative method from [13] is used for homogenization of reflectors.

The P1 equation of the first moment for the 1D geometry is written as:

$$\frac{1}{3}\frac{\partial \phi_g(z)}{\partial z} + \Sigma_{t,g} J_g(z) = \sum_{g'=1}^{G} \Sigma_{s,1,g'\to g} J_{g'}(z) \tag{11}$$

Using Fick's law, Eq. (11) can be rewritten as:

$$\frac{1}{3}\frac{\partial \phi_g(z)}{\partial z} - \Sigma_{t,g} D_g \frac{\partial \phi_g(z)}{\partial z} = -\sum_{g'=1}^{G} \Sigma_{s,1,g'\to g} D_{g'} \frac{\partial \phi_{g'}(z)}{\partial z} \tag{12}$$

The integration of Eq. (12) can obtain:

$$\frac{1}{3}\phi_g - \Sigma_{t,g} D_g \phi_g = -\sum_{g'=1}^{G} \Sigma_{s,1,g'\to g} D_{g'} \phi_{g'} \tag{13}$$

After MC calculation, the quantities except for the diffusion coefficient are known, so we can solve the linear equation of Eq. (13) to calculate diffusion coefficient.

2.3 Leakage Correction

As described before, the leakage correction is necessary for homogenization since the infinite assembly differs from its actual condition in the critical core. In spite of it that some approaches like the buckling-search [14] and the albedo-search method [15] have been developed for MC, the leakage correction in NECP-MCX follows the homogeneous fundamental mode approximation [1] in the deterministic lattice physics code since its efficiency and successful application.

Using the modal expansion method, the flux in a 1D system can be expanded using its fundamental approximation which assumes that space- and energy-dependence can be separated:

$$\phi(z, E, \mu) = \psi(z)\varphi(E, \mu) \tag{14}$$

where $\psi(z)$ describes the spatial dependence, and is the spectrum.

The spatial term $\psi(z)$ satisfies the wave equation:

$$\nabla^2 \psi(z) + B^2 \psi(z) = 0 \tag{15}$$

where $B^2\varphi(E, \mu)$ is the buckling.

Then we can obtain:

$$\psi(z) = \psi_0 e^{\pm iBz} \tag{16}$$

Based on Eq. (14), Eq. (16), the 1-order expansion of anisotropic scattering, and the 1D neutron transport equation, we can obtain the B1/P1 equations:

$$\begin{aligned} &\Sigma_t(E)\varphi(E) \pm iBJ(E) = \\ &\int_0^\infty dE' \Sigma_{s,0}\left(E' \to E\right)\varphi\left(E'\right) + \chi(E) \\ &\pm iB\varphi(E) + 3\alpha[B, \Sigma_t(E)]\Sigma_t(E)J(E) = \\ &3\int_0^\infty dE' \Sigma_{s,1}\left(E' \to E\right)J\left(E'\right) \end{aligned} \tag{17}$$

The difference of B1 and P1 equations is $\alpha[B, \Sigma_t(E)]$. For B1 equation:

$$\alpha[B, \Sigma_t(E)] = \begin{cases} \frac{1}{3}x^2\left(\frac{\arctan(x)}{x - \arctan(x)}\right), & x^2 = (B/\Sigma_t(E))^2 > 0 \\ \frac{1}{3}x^2\left(\frac{\ln\left(\frac{1+x}{1-x}\right)}{\ln\left(\frac{1+x}{1-x}\right) - 2x}\right), & x^2 = -(B/\Sigma_t(E))^2 > 0 \end{cases} \tag{18}$$

For P1 equation:

$$\alpha[B, \Sigma_t(E)] = 1 \tag{19}$$

The critical spectrum can be calculated by solving Eq. (17) with changing buckling iteratively until the eigenvalue converges to 1. Then, the multigroup flux is corrected by the critical spectrum for further treatments.

2.4 Assembly Discontinuous Factor

The strict definition for ADF is as Eq. (6), but approximated calculations must be performed for Eq. (6) since the surface flux of the assembly in neither the heterogeneous nor the homogeneous core is unknown.

For the homogenization of infinite assembly, the heterogeneous surface flux is approximated by the surface flux from the infinite assembly transport calculation, and the homogenized surface flux is approximated by the volume-averaged flux from the infinite assembly transport calculation since the flux in the homogenized region is constant under zero net current. The ADF is calculated as:

$$f_{g,k} = \frac{\phi_{g,k}^A}{\overline{\phi}_g^A} \tag{20}$$

For the homogenization of problems without zero net current, the approximation of heterogeneous surface flux follows Eq. (20), but the approximation of homogenized surface flux in Eq. (20) fails since the flux in such a homogenized region is inconstant. Therefore, it is important to calculate a homogenized diffusion flux using the same diffusion calculation method as the downstream nodal diffusion code.

2.5 Overall Calculation Flow

The overall calculation flow for the MC homogenization is given below (Fig. 1).

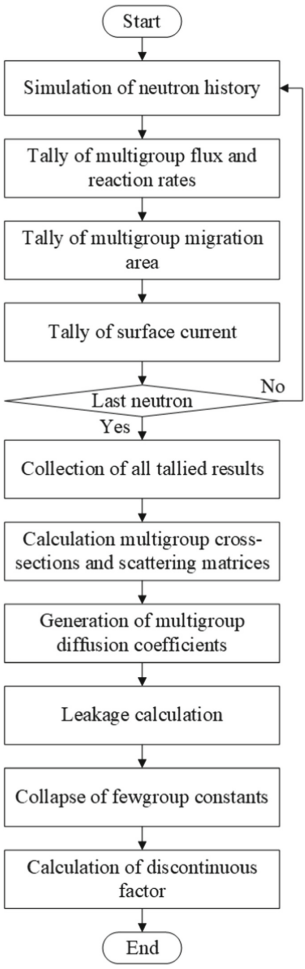

Fig. 1. Overall calculation flow for the MC homogenization

3 Verification

The validity of few-group constants generated by NECP-MCX is verified in this section. A code sequence called MCX-SPARK, where NECP-MCX generates the few-group constants and SPARK [16] performs the nodal diffusion calculation, is built for the two-step calculation. The reference results are from the design report and Bamboo-C [16]. Bamboo-C is a home-developed PWR fuel management software and has undergone the engineering validations of commercial PWR for over 100 reactor years.

The physics start-up test of HPR1000 [9] is simulated using MCX-SPARK for verification. HPR1000 is a Chinese design of the third-generation commercial PWR. There are five control rod banks in the HPR1000 notated by G1, G2, N1, N2, R, and three shutdown banks notated by SA, SB, and SC. Several tests including the critical boron concentration and the isothermal temperature coefficient under insertion of different control rods are simulated. Different control rod bank worths are also calculated.

For MC homogenization of the fuel assemblies, the quarter models of different fuel assemblies, which are classified by the fuel enrichment, the burnable absorber, the control rods, and the grid spacer, are built. A total 500 cycles including 100 inactive cycles with 200 000 particles per cycle are adopted. For the homogenization of the reflectors, the one-dimensional reflector models are built with two models for the top and bottom reflectors and nine models for the radial reflectors according to their positions. A total 500 cycles including 100 inactive cycles with 500 000 particles per cycle are adopted for the homogenization of reflectors.

3.1 Critical Boron Concentration

The tests for critical boron concentration under 11 different states are simulated and Table 1 gives the comparison of critical boron concentrations calculated by MCX-SPARK to the reference results.

Table 1. Comparison of critical boron concentration

State	Bias with the design report (ppm)	Basic with Bamboo-C (ppm)
All rods out (ARO)	−31.256	−6.473
R in	−30.635	−5.996
R, G1 in	−31.854	−6.272
G1 in	−31.411	−6.487
G1, G2 in	−33.72	−6.450
G1, G2, N1 in	−38.147	−7.501
G1, G2, N1, N2 in	−30.488	−3.165
R, G1, G2, N1, N2 in	−28.136	−0.761
R, G1, G2, N1, N2, SC in	−31.025	−1.950
R, G1, G2, N1, N2, SC, SB in	−34.483	−4.344
All rods in (ARI) with the R rod at B08 out	−45.415	−7.959

It can be seen from Table 1 that the bias between the MCX-SPARK and the design report is −45 to −28 ppm, which satisfies the limit of 50 ppm. The bias between the MCX-SPARK and Bamboo-C is −8 to −1 ppm, which has a good agreement.

3.2 Isothermal Temperature Coefficient

The isothermal temperature coefficient is a reflector of both the moderator temperature coefficient and the fuel Doppler temperature coefficient, and it is an important content in the physics start-up test. Three states are calculated and compared. Table 2 gives the results.

Table 2. Comparison of isothermal temperature coefficient

State	Bias with the design report (pcm/°C)	Bias with Bamboo-C (pcm/°C)
ARO	−0.337	0.048
R in	−1.035	0.008
R, G1 in	−1.069	−0.037

The bias between the MCX-SPARK sequence and the design report is −1.069 to −0.337 pcm/°C, which satisfies the limit of 3.6 pcm/°C. The bias of three isothermal temperature coefficients between MCX-SPARK and Bamboo-C is less than 0.1 pcm/°C.

3.3 Control Rod Bank Worth

Different control rod banks worth values measurement by boron dilution method or rod swap method in the physics start-up test are also simulated using MCX-SPARK sequence, and the comparison of the results are given in Table 3.

Table 3. Comparison of control rod bank

Test item	Bias with the design report (%)	Bias with Bamboo-C (%)
Worth of R by boron dilution	0.2	−0.3
Worth of G1 by boron dilution with R in	4.7	0.9
Worth of SB by boron dilution	−0.7	−0.4
Worth of SA by rod swap	0.1	−0.8
Worth of N2 by rod swap	−1.8	−1.7
Worth of N1 by rod swap	1.6	0.5
Worth of G2 by rod swap	0.1	−0.1
Worth of SC by rod swap	1.9	1.3
Worth of G1 by rod swap	−0.2	0.2
Worth of SB rods by rod swap at G03 and J13	0.9	−0.1

(*continued*)

Table 3. (*continued*)

Test item	Bias with the design report (%)	Bias with Bamboo-C (%)
Worth of SB rods at G13 by rod swap	1.5	0.4
Worth of G1 by boron dilution	3.2	0.2
Worth of G2 by boron dilution with G1 in	2.9	0.1
Worth of N1 by boron dilution with G1, G2 in	6.4	1.6
Worth of N2 by boron dilution with G1, G2, N1 in	−3.0	−2.1
Worth of R by boron dilution with G1, G2, N1, N2 in	−1.2	−1.1
Worth of SC by boron dilution with R, G1, G2, N1, N2 in	4.4	1.6
Worth of SB by boron dilution with R, G1, G2, N1, N2, SC in	2.3	2.0

The range of bias for the MCX-SPARK and design report is −2.989 to 6.442%, with the RMS bias of 1.692%, which satisfies the limit of 10%. The results of the MCX-SPARK agree well with Bamboo-C, with the bias being −2.084 to 1.981%, and the RMS bias being 0.521%.

4 Conclusion and Discussion

In this study, the Monte Carlo code NECP-MCX is extended to generate the assembly-homogenized few-group constants. The cumulative migration method is used to generate the diffusion coefficient with minimum approximation and the leakage correction is performed using the fundamental mode approximation. A two-step code sequence named MCX-SPARK is built based on MC homogenization. The physics start-up test of HPR1000 is simulated by this code sequence. The results are compared with the design report and a deterministic PWR fuel management software Bamboo-C. It is observed that the biases of all test items between the MCX-SPARK and the design report satisfy the limit value. In addition, MCX-SPARK also agrees well with Bamboo-C.

The capability of NECP-MCX for the generation of few-group constants is developed and verified. But it should be noted that the application of this capability in this study is PWR two-step calculation, which poses almost no particular difficulty for current deterministic lattice physics code. In spite of it, this study, which shows the validity of MC homogenization for the practical application, gives a perspective of MC homogenization for further practical application of reactors where many approximations must be made for deterministic lattice physics calculation.

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