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Application of the hyperfine group self-shielding calculation method to the lattice and whole-core physics calculation

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ABSTRACT

The hyperfine group method is considered as the most accurate resonance self-shielding method, but it suffers some limitations in the practical calculation due to its long computation time. In order to make it practical to use the hyperfine group method in large scale geometry problems, a cross section interpolation method is proposed in the frame of the newly developed global-local self-shielding method. In this paper, a series of typical 1-D pin cells are established by varying the Dancoff correction factor, burnup depth and fuel temperature. The hyperfine group method is just performed to these typical pin cells, and the cross sections of the realistic pin cells are obtained by interpolating according to the real values of these parameters. By this method, the times of the hyperfine group method needed to be performed is greatly reduced. This method has a very high accuracy in practical assembly and whole-core physics calculation.

1. Introduction

In the deterministic nuclear reactor physics analysis, the multi-group treatment for the energy variable in neutron transport equation is a basic technique to make the transport calculation feasible. Consequently, the resonance self-shielding calculation is necessary to obtain the multi-group effective cross sections in the resonance energy range, and its accuracy has important impact on the following transport calculation. The resonance self-shielding calculation is a complicated work, due to the phenomena caused by the sharply varied resonance cross sections, including the spatial self-shielding effect, Doppler effect and interference among different resonant isotopes. In order to simplify the calculations, the above mentioned effects are usually approximately treated in the conventional resonance self-shielding methods.

The equivalence theory (Stamm'ler and Abbate, 1983) and subgroup method (Nikolaev et al., 1970) are the widely used resonance self-shielding methods in the modern lattice physics codes, due to their high computation efficiency. In the equivalence theory, the fuel is treated as a lump, so only the average cross sections over the whole fuel rod can be obtained. In order to account for the spatial self-shielding effect in the fuel rod, the Space-Dependent Dancoff Method (SDDM) is proposed by Matsumoto et al. (2005), and then it is extended to account for the radial temperature distribution within a fuel rod (Matsumoto et al., 2006). In the subgroup method, the spatial self-shielding effect can be directly treated by solving the subgroup transport equation with fine spatial meshes in the fuel rod, however, it is hard to treat the nonuniform temperature distribution in the fuel rod. For this reason, the weight adjustment scheme and number density adjustment scheme are proposed to solve this problem (Joo et al., 2005; Jung et al., 2016; Wemple et al., 2007). A partial cross section fitting scheme is proposed to treat the nonuniform temperature by fitting cross sections at different temperatures as partial cross sections (He et al., 2018). Moreover, the equivalence theory and subgroup method suffer a long-standing issue, i.e. the resonance interference effect (Williams, 1983). The Bondarenko iteration method is the common method to treat the resonance interference effect, and an alternative is the resonance interference factor (RIF) method (Williams, 1983). Recently, a new method called pseudo-resonant isotope method has been proposed by the research group of the authors (Zu et al., 2016), where the resonance integral (RI) table of a mixture of resonant isotopes is used instead of providing individual RI table for each isotope, and the interference effect is inherently included in RI table.

In order to enhance the safety and economy of nuclear reactors, the neutronics analysis with higher accuracy has long been pursued, either in the conventional nodal diffusion based methods, or in the whole-core direct neutronics simulation. Therefore, more accurate resonance self-shielding method should be researched to satisfy various demands. The hyperfine group method is consid-

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ered as the most accurate resonance self-shielding method. In theory, the hyperfine group method can avoid all the drawbacks of equivalence theory and subgroup method, by directly solving the neutron slowing-down equation using hyperfine group cross sections of each isotope at the realistic temperature within each spatial mesh. However, a large computational resource is required to perform hyperfine group resonance calculation, so that it is hardly applied to analyze a 2-D problem, such as an assembly or even a 2-D pin cell, and it is just limited to 0-D or 1-D problem.

In the past, the hyperfine group method was usually used to produce correction factors to improve the accuracy of conventional equivalence theory and subgroup method, for example, the RIF is obtained by performing 0-D hyperfine group calculations. Recently, some efforts have been made to directly apply the hyperfine group method to produce effective self-shielded cross sections for a large scale problem. The present paper will review some works applying the hyperfine group method, and then propose a practical method to apply the hyperfine group method to the lattice physics and direct whole-core neutronics simulations.

This paper is organized as follows. In Section 2, the basic methodology of hyperfine group method is briefly described; some recent works to improve the hyperfine group method are reviewed, and then an interpolation method is proposed to enhance the practical application of the hyperfine group method in the lattice and whole-core physics simulations. In Section 3, the proposed method is tested against the several benchmarks. Some conclusions are given in the last sections.

2. Methodologies

2.1. Hyperfine group method

The continuous energy neutron slowing-down equation in collision probability format is usually used in the hyperfine group method, which is given as follows:

$$\Sigma_{t,i}(E)\phi_i(E)V_i = \sum_j P_{j\to i}(E)V_j\left(\begin{array}{c}\int_0^\infty \Sigma_{s,j}(E'\to E)\phi_j(E')dE' \\ +\chi_j(E)\int_0^\infty \nu\Sigma_{f,j}(E')\phi_j(E')dE'\end{array}\right), \quad (1)$$

where i is the index of spatial meshes; $\Sigma_{t,i}(E)$ is the macroscopic total cross section; $\phi_i(E)$ is the neutron scalar flux; V_i is the volume; $P_{j\to i}(E)$ is the collision probability from region j to i; $\Sigma_{s,i}(E'\to E)$ is the macroscopic scattering cross section from energy E' to E; $\chi_i(E)$ is the fission spectrum; $\nu\Sigma_{f,i}(E')$ is the macroscopic production cross section.

In Eq. (1), the energy variable is discretized into hyperfine groups, and the energy interval of a group should be narrow compared with the maximum energy lose per scattering of the heaviest isotope. Therefore, the neutron flux and cross section within a fine energy group can be thought to be constant. Besides, the fission source in the resonance energy range can also be ignored without introducing apparent error. Eq. (1) is leaded to the following form:

$$\Sigma_{t,i,fg}\phi_{i,fg}V_i = \sum_j P_{j\to i,fg}V_j S_{j,fg}, \quad (2)$$

where fg is the index of hyperfine groups; $\Sigma_{t,i,fg}$ is the macroscopic total cross section of group fg; $\phi_{i,fg}$ is the neutron scalar flux of group fg; $P_{j\to i,fg}$ is the collision probability from region j to i of group fg; $S_{j,fg}$ is the scattering source of group fg in region j.

In resonance energy range, it can be assumed that the slowing-down of neutrons is dominated by the elastic scattering, and the asymptotic scattering kernel is used to describe the energy distribution of scattered neutrons. The source term $S_{j,fg}$ in Eq. (2) can be written as:

$$S_{j,fg} = \sum_k \sum_{fg'} \frac{\Sigma_{es,j,k,fg'}\phi_{j,fg'}\Delta E_{fg'}}{(1-\alpha_k)E_{fg'}} \quad (3)$$

and

$$\alpha_k = \left(\frac{A_k-1}{A_k+1}\right)^2 \quad (4)$$

where k is the isotope index; j is the index of spatial meshes; $\Sigma_{es,j,k,fg'}$ is the macroscopic elastic scattering cross section; $\phi_{j,fg'}$ is the neutron scalar flux; $\Delta E_{fg'}$ is the energy interval of group fg'; A_k is the mass of nuclide k relative to that of the neutron.

Once the neutron flux of the hyperfine group is obtained, the multi-group effective cross sections of each nuclide are calculated by:

$$\sigma_{x,i,g} = \frac{\sum_{fg\in g}\phi_{i,fg}\sigma_{x,i,fg}}{\sum_{fg\in g}\phi_{i,fg}} \quad (5)$$

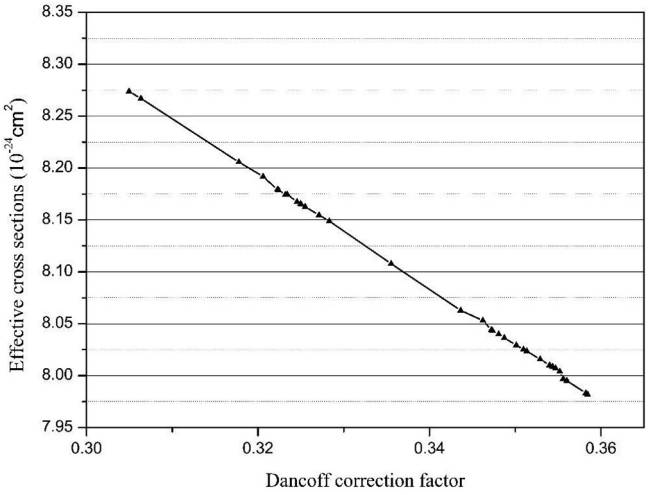

Fig. 1. Multi-group effective absorption cross sections of group 27 for U-238 versus Dancoff correction factors.

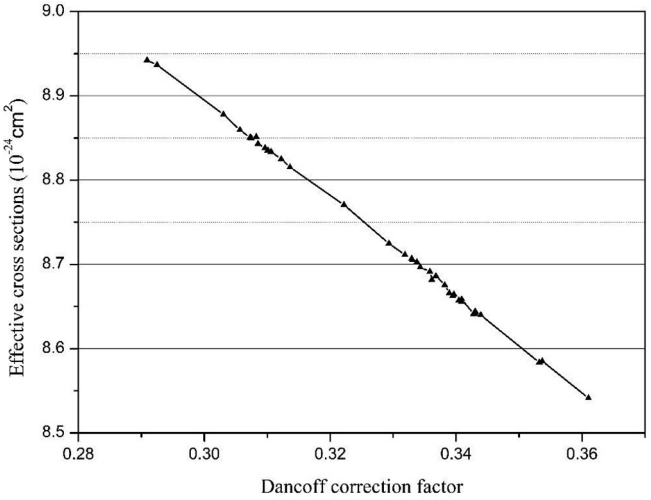

Fig. 2. Multi-group effective absorption cross sections of group 27 for U-238 versus Dancoff correction factors at the burnup of 40 GWd/tU.

where i is the region index; g is the multi-group index; $\sigma_{x,i,g}$ is the microscopic multi-group effective cross section of reaction type x; $\sigma_{x,i,fg}$ is the microscopic cross section of hyperfine group fg.

The hyperfine group method is favorable when the multi-group effective cross sections of high precision and resolution are desired. But the practical application of the hyperfine group method is limited to 0-D or 1-D problem, due to its great demand for computation resource. There are two main factors affecting the calculation efficiency. The first is the calculation of collision probabilities shown in Eq. (2). The collision probability between any two regions at each energy group should be calculated before solving the slowing-down equation. For each energy group, the amount of collision probabilities needing to be calculated is proportional to the square of the region number, so that when the system contains a large number of spatial meshes, the computational efficiency is significantly decreased. Moreover, it is also very complicated to calculate the collision probabilities in a complex geometry. The second factor is the calculation of scattering source. As shown in Eq. (3), the scattering source for an energy group is calculated by summing up the contribution of all the higher energy groups that can transfer into this energy group. The range of the higher energy can be very large for the light isotopes, especially when the hydrogen is contained in the material. Thus, the computational cost will be very large, if the scattering source is directly calculated according to Eq. (3). Besides, the scattering source should also sum up the contribution of all the isotopes in the material. In the burnt fuel, there are hundreds of fission products, so the computational time will also increase in this case. The following subsections, some efforts made to apply the hyperfine group method are reviewed, and a new interpolation method is proposed to enhance the practical application of the hyperfine group method.

2.2. Treatment of the collision probability

For a specific problem, the collision probabilities among different regions can be classified into two categories. The first is the collision probabilities among the subregions within a fuel rod. The spatial self-shielding effect is taken into account through this type of collision probabilities. The second is the collision probabilities between a subregion in a fuel rod and a region outside the fuel rod including moderator and other fuel rods. This type of collision probabilities incorporates the shadow effect into the effective cross sections.

Considering the feasibility, the hyperfine group method is usually used to treat a 1-D problem. In a 1-D cylindrical fuel pin, if the fuel pin is divided into multiple rings, the collision probabilities among different regions can be rigorously calculated using the Carlvik method (Carlvik, 1964), based on the realistic temperature and material composition in each spatial region. In this situation, the rings are treated as different regions. In the next section, we will show that when the fuel rod is divided into ten rings, the time for calculating the collision probabilities is about 4.4 s. If a system such as an assembly includes hundreds of fuel rods, the time for the resonance self-shielding calculation is unacceptable. Therefore, some efforts have been made to enhance the feasibility. A method is proposed in the work (Liu et al., 2015) to approximately calculate the region-to-region collision probability $P_{i\to j}(E)$ when the non-uniform distribution of material composition and temperature along the radial direction in the fuel rod is accounted for, as follows:

$$P_{i\to j}(E) \approx P_{i\to j}^{T_i,C_i}(E)\frac{1-P_{esc,i}(E)}{1-P_{esc,i}^{T_i,C_i}(E)} \tag{6}$$

where, $P_{i\to j}^{T_i,C_i}(E)$ is the collision probability from region i to j assuming a uniform temperature and material composition throughout the whole fuel rod; the $P_{esc,i}(E)$ is the escape probability of a neutron born in region i, calculated with the realistic temperature profile and material composition; $P_{esc,i}^{T_i,C_i}$ is the escape probability of the situation with a uniform temperature and material composition in the fuel rod.

In Eq. (6), with the assumption of a uniform temperature and material composition, the $P_{i\to j}^{T_i,C_i}(E)$ can be calculated in advance and tabulated as a function of total cross section levels, and then

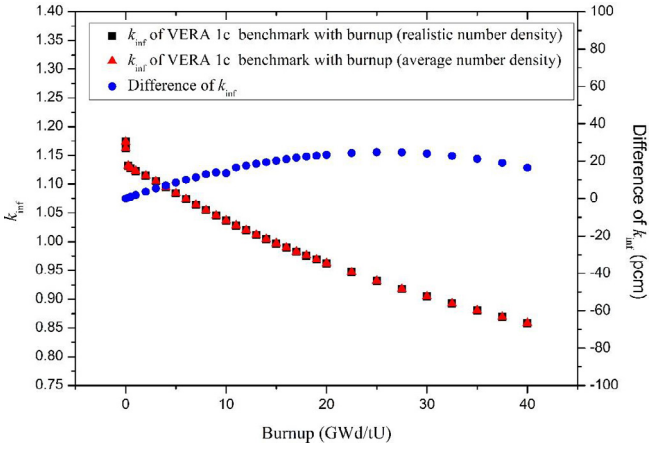

Fig. 3. Comparison of k_{inf} of VERA 1C burnup benchmark with realistic number density and average number density.

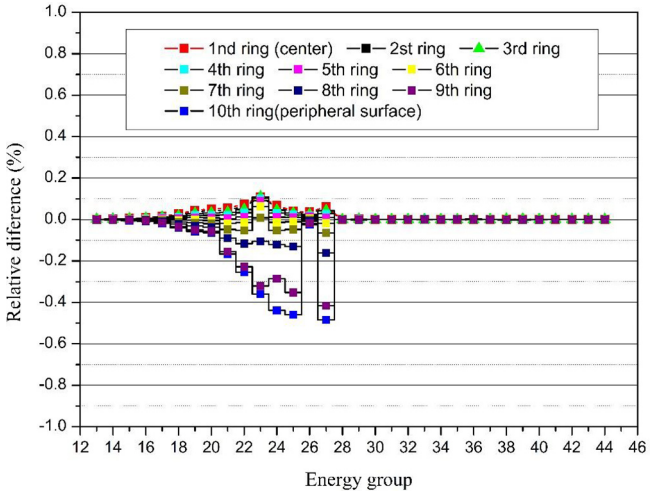

Fig. 4. Comparison of effective absorption cross section for U-238 of VERA 1C burnup benchmark with realistic number density and average number density.

Table 1
Temperature profile of test case.

Ring number	Radius (cm)	Temperatures of case (K)
1 (center)	0.12953	1170
2	0.18318	1110
3	0.22435	1050
4	0.25905	990
5	0.28963	930
6	0.31727	870
7	0.34270	810
8	0.36636	750
9	0.38858	690
10 (peripheral surface)	0.40960	630

Table 2
Calculation time for pin cell.

	Temperature distribution	Number density distribution	Total time (s)	Pre-process time (s)	Source term calculation time (s)	Collision probability calculation time (s)
Case 1	No	No	0.38	0.22	0.03	0.13
Case 2	Yes	No	4.89	0.42	0.03	4.44
Case 3	No	Yes	7.11	1.50	1.08	4.53

in the realistic calculation, the values of collision probabilities can be interpolated according the total cross section of the fuel. This is very helpful to increase the calculation efficiency.

In order to incorporate the shadow effect, the escape probabilities $P_{esc,i}(E)$ is further expressed as follows:

$$P_{esc,i}(E) = \frac{\Sigma_{e,i}(E)}{\Sigma_{t,i}(E) + \Sigma_{e,i}(E)} \tag{7}$$

where, $\Sigma_{e,i}(E)$ is the escape cross section which is gotten by rigorously evaluating $P_{esc,i}(E)$ using Carlvik method based on the realistic fuel temperature profile and material compositions in an isolated 1-D pin which is a fuel rod surrounding with infinite moderator, and then is modified by a factor to incorporate the shadow effect (Liu et al., 2015).

The above procedure is tedious, so that in the lattice code STREAM (Choi et al., 2017), a different method is used to incorporate the shadow effect. In this method, $P_{esc,i}(E)$ is evaluated as follows:

$$P_{esc,i}(E) = \eta_i P^{iso}_{esc,i}(E) \tag{8}$$

where, $P^{iso}_{esc,i}(E)$ is the escape probability of subregion i in an isolated pin; η_i is called shadow effect correction factor, and obtained as:

$$\eta_i = \frac{P_{esc,F}(\Sigma_{t,F})}{P^{iso}_{esc,F}(\Sigma_{t,F})} \tag{9}$$

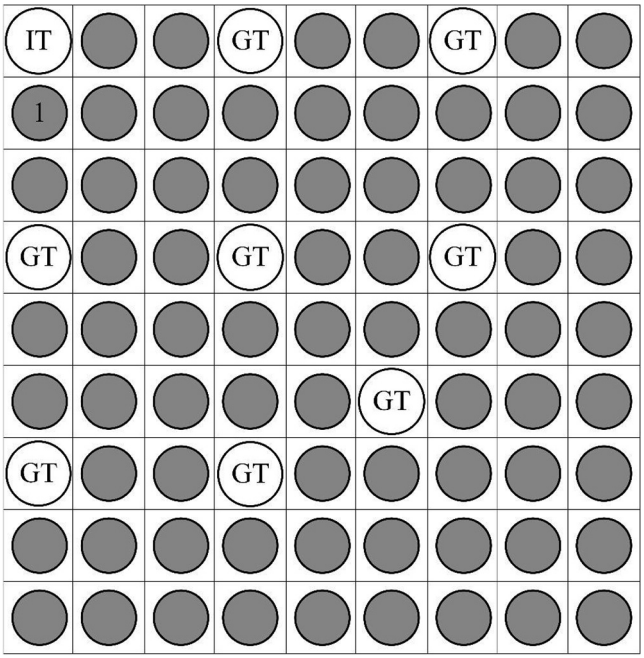

Fig. 5. Geometry of VERA 2C problem.

Table 3
Infinite multiplication factor of VERA 2C benchmark.

Reference k_{inf}	Calculated k_{inf}	Difference of k_{inf} (pcm)
1.17375 ± 0.00002	1.17482	107

The $P_{esc,F}(\Sigma_{t,F})$ and $P^{iso}_{esc,F}(\Sigma_{t,F})$ are the escape probabilities respectively for the realistic geometry and the isolated pin. The two escape probabilities are evaluated using the Carlvik's two term rational approximation with assuming a uniform total cross section $\Sigma_{t,F}$ in the fuel region. The two term rational expression of $P_{esc,F}(\Sigma_{t,F})$ involves the Dancoff factor which represents the shadow effect and is calculated by the neutron current method (NCM) (Sugimura and Yamamoto, 2006). The NCM just performs one-group fixed source transport calculations, and it is efficient to get the Dancoff factor.

Recently, the research group of the authors has proposed a new method called global-local self-shielding calculation method to account for the shadow effect (Liu et al., 2018). In this method, an equivalent 1-D cylindrical pin cell is established to represent the realistic pin cell in a assembly. The Dancoff correction factor for each realistic pin cell in the analyzed system is evaluated by the NCM. After getting the Dancoff correction factor, the equivalent 1-D cylindrical pin cell is established by adjusting the moderator radius to make the Dancoff correction factor in the two system equal. The relation between the moderator radius and the Dancoff correction factor in a 1-D pin cell is as follows:

$$C = \frac{P^{iso}_{esc,F} - P_{F\to M}(R)}{\Sigma_{t,F} l P_{F\to M}(R) + P^{iso}_{esc,F} - P_{F\to M}(R)} \tag{10}$$

where, $P^{iso}_{esc,F}$ is the escape probability for an isolated fuel rod; $P_{F\to M}(r)$ is the collision probability from the fuel to moderator in the 1-D cylindrical pin cell whose moderator radius is R; $P^{iso}_{esc,F}$ and $P_{F\to M}(r)$ are evaluated with Carlvik method by assuming a uniform total cross section of $\Sigma_{t,F}$ in the fuel rod; l is the average chord length of the fuel rod.

In the lattice code GALAXY (Yamaji et al., 2018), a similar method with that proposed by the authors is used to realize practical application of the hyperfine group method in the lattice physics calculations. Besides, in another work of the authors, the embedded self-shielding method is adopted to establish the 1-D equivalent 1-D pin cell (Zu et al., 2018). The difference between global-local self-shielding calculation method and the method proposed by Yamaji et al. (2018) is the method used to calculate Dancoff factor. The method proposed by Yamaji et al. (2018) obtains Dancoff factor by the enhanced neutron current method (ENCM) and IR approximation. The global-local self-shielding calculation method obtains Dancoff factor in lattice by NCM and Dancoff factor in 1-D pin cell by collision probability.

The equivalent 1-D cylindrical pin cells are independent on each other, so any resonance self-shielding method can be applied to the equivalent pin cells. Although the hyperfine group method can be directly carried out on each pin cell, it is still unpractical for a large scale problem, because there is a large amount of equivalent pin

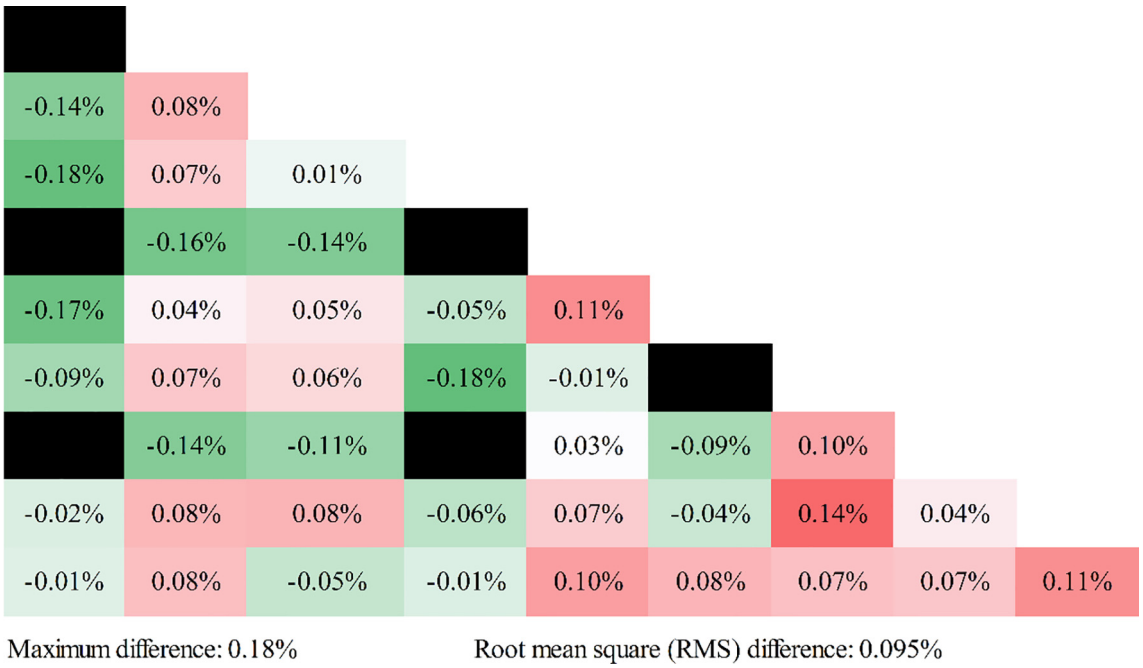

Fig. 6. Comparison of pin powers for VERA 2C benchmark.

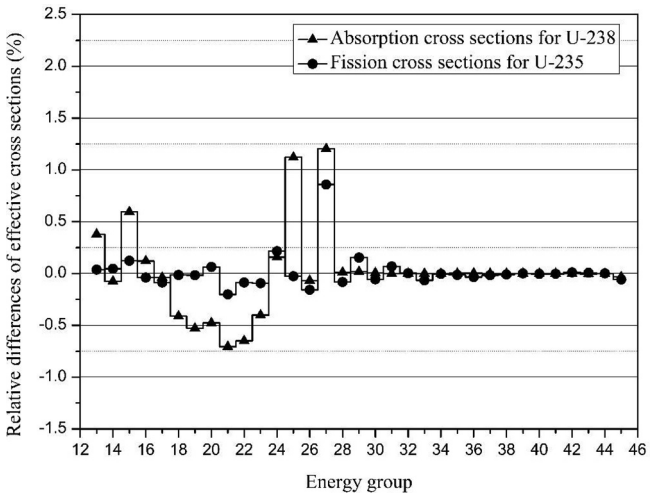

Fig. 7. Comparison of effective cross sections of fuel pin 1 in VERA 2C benchmark.

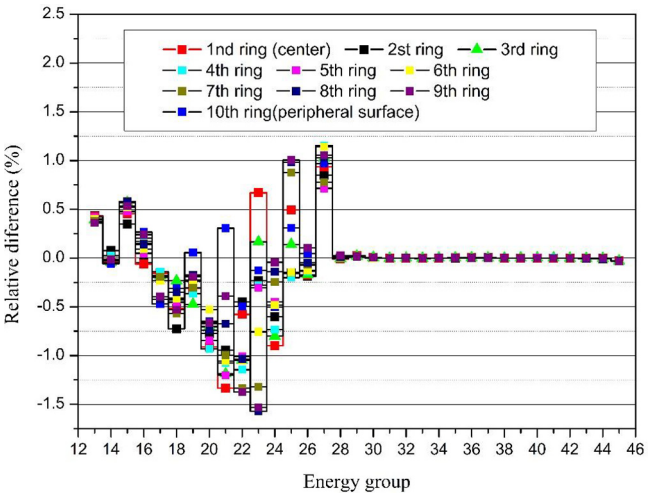

Fig. 8. Comparison of effective cross sections for U-238 of fuel pin 1 in VERA 2C benchmark.

cells needing to be calculated. Therefore, in the previous work (Liu et al., 2018), the sub-group method using a pseudo-resonant-isotope RI table is adopted to the 1-D pin cells.

2.3. Treatment of the scattering source

For the calculation of the scattering source in Eq. (3), the simplest method is using the narrow resonance (NR) approximation or intermediate resonance (IR) approximation. However, the previous work has shown that the NR or IR approximation can introduce large errors into the multi-group effective cross sections (Zhang et al., 2015). In the work (Sugimura and Yamamoto, 2007), the NR approximation is only used in the moderator region, and the scattering source of fuel regions is rigorously evaluated.

Instead of directly implementing Eq. (3), the scattering source can be effectively calculated by a recursive formula. In the RMET code and CENTRM module of SCALE, two different recursive formulae are derived based on different energy discretization methods. In REMT, the energy range is divided into a large number of equal-lethargy groups (Leszczynski, 1987), while in CENTRM, the interval of each mesh is non-uniform and problem-dependent (Williams and Asgari, 1995).

The recursive formulae can significantly reduce the amount of required computation for the scattering source of a nuclide. However, in the burnt fuel, there are hundreds of fission products, the total scattering source should sum up all the nuclides in the fuel. It also takes a long time in this situation.

2.4. An interpolation method to accelerate the hyperfine group method

As mentioned above, although the Dancoff correction factor equivalence method can decouple a large system into independent fuel pins and the recursive formulae can also accelerate the calcu-

lation of scattering source, it is still need much time if all the independent equivalent fuel pins are calculated using the hyperfine group method. Therefore, an interpolation method is proposed to reduce the number of times that the hyperfine group calculations are performed.

For a running reactor, when the operation status is changed, two parameters will vary and have important impact on the multi-group effective cross sections, i.e. the fuel temperature and moderator density. Besides, the material composition of nuclear fuel is changing during the operation of a reactor, which is another important factor needing to be considered. Here, it is worth mentioning that according to the conventional equivalence theory, the moderator density directly affects the shadow effect (Knott and Yamamoto, 2010), so the Dancoff correction factor which is used to represent the shadow effect in equivalence theory is applied instead of the moderator density. Therefore, a cross section interpolation method versus the variables of fuel temperature, Dancoff correction factor and burnup depth is proposed to reduce the amount of computation. Taking an assembly problem as example, the detailed procedure of the interpolation method is described as follows.

The NCM is firstly carried out on the assembly to obtain the Dancoff correction factor for each pin in the system. According to the range of the values of Dancoff correction factors, several typical values of the Dancoff factor are chosen to establish the equivalent 1-D pin cells. The equivalent 1-D pin cells with different radius are constructed by preserving the Dancoff correction factors. In this step, the fuel temperature and material composition have no impact on the value of Dancoff correction factor, because the fuel is treated as black in the NCM, and in the actual calculation, the total cross section of nuclear fuel is set to be 10^5 cm^{-1}. After getting the radius of the equivalent 1-D pin cells, the fuel temperature and material composition in the fuel rods should be defined before performing the hyperfine group calculations. Here, the fuel temperature uses the average value of the fuel, and the material composition also uses the average value determined according to burnup calculation. As the Dancoff correction factor, several typical values are respectively chosen for these two parameters according to the realistic distribution.

Based on the above treatment, a series of typical equivalent 1-D pin cells are obtained, and then the hyperfine group resonance calculations are carried out on each pin cell. The effective cross sections of the typical equivalent fuel rods are used to construct an interpolation table, and the cross sections of all the realistic pin cell in the assembly are gotten by interpolating the table versus their Dancoff correction factor, fuel temperature and burnup depth.

There are two factors should be demonstrated here. The first is the number of the typical values of the three parameters and the corresponding interpolation methods. In order to illuminate the relation between the cross sections and interpolation variables, the VERA 2C benchmark is analyzed. The multi-group structure used in the present paper is WIMSD 69 group format. The range of resonance-energy group is from group 13–45. The energy range of the group 27 is 4 eV – 9.877 eV. The multi-group effective absorption cross sections of group 27 for U-238 versus Dancoff correction factors is shown in Fig. 1. It is obvious that the effective cross section varies linearly with Dancoff correction factors. So the linear interpolation method is used for the Dancoff correction factors using three interpolation points. The multi-group effective absorption cross sections of group 27 for U-238 at 40 GWd/tU versus Dancoff correction factors is shown in Fig. 2. It can be seen that the effective cross section varies almost linearly with Dancoff correction factors and fluctuates slightly because of burnup. So the linear interpolation method is also used for the burnup depth using three interpolation points. The square root-linear interpolation is usually adopted for the fuel temperature (Knott and Yamamoto, 2010), so that this interpolation method is also employed in the present work. Three interpolation points are chosen in the calculations, because the average fuel temperature changes slightly in an assembly.

The second factor is how to get the spatially dependent cross sections within a fuel rod. The radial distributions of material composition and temperature in the fuel pellet, and the spatial self-shielding effect affect the cross section distribution along the radial direction. In the above described interpolation procedure, a uniform material composition and fuel temperature is assumed to realize the interpolation scheme of effective cross section. For the material composition, the numerical results show that if the uniform number density is used in the resonance self-shielding calculation, while the realistic number densities in each subregions is used in the burnup calculation, the infinity multiplication factor (k_{inf}) and effective cross section show little deviation from the results gotten by using the realistic number densities to perform self-shielding calculation. The VERA 1C benchmark is calculated to justify this phenomenon, and the results are shown in Figs. 3 and 4. In order to show the effect of using a uniform number density to perform the self-shielding calculations on the spatially dependent cross sections, the fuel rod is divided into 10 rings by equal volume. It can be seen that the difference of k_{inf} is less than

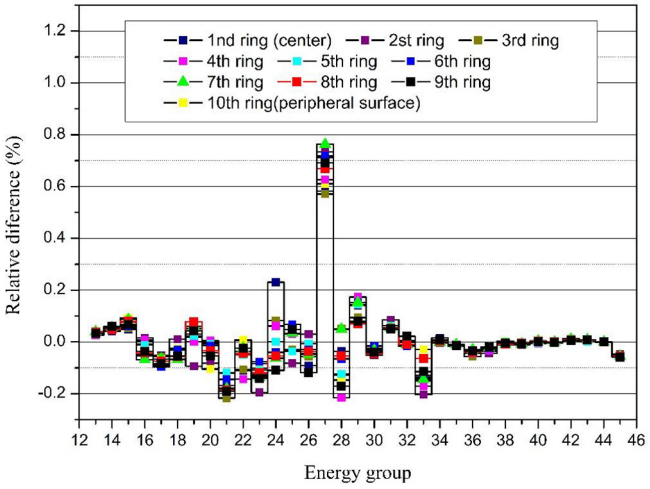

Fig. 9. Comparison of effective cross sections for U-235 of fuel pin 1 in VERA 2C benchmark.

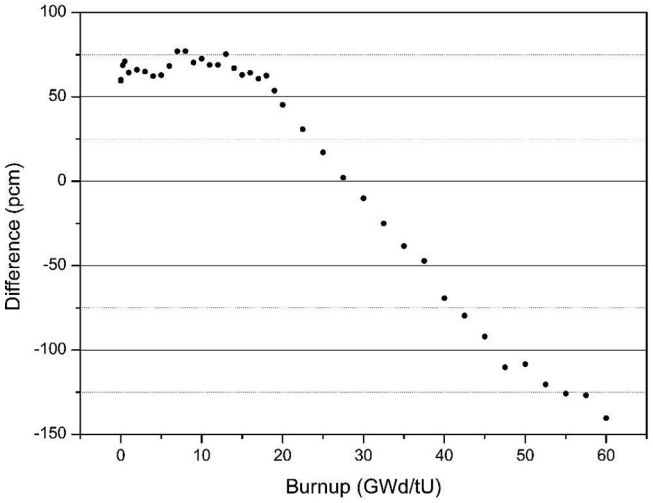

Fig. 10. Comparison of k_∞ vs burnup in VERA 2D benchmark.

30 pcm, and the absolute values of the differences of effective cross sections are less than 0.6%. Therefore, the uniform material composition is used in the resonance self-shielding calculation. For the fuel temperature, if the fuel temperature profile in a fuel rod is considered in the resonance self-shielding calculation, each ring should be treated as a different region, so that it will take much time to calculate the collision probabilities. Therefore, the fuel temperature distribution is not considered in the present paper, and the effective fuel temperature is used in the calculations. As for the spatial self-shielding effect, the spatially dependent cross sections within a fuel rod can be obtained by the proposed interpolation method, after the spatially dependent cross sections are obtained in the typical equivalent pin cells.

3. Numerical results

The above described method has been implemented into the high-fidelity neutronics code NECP-X (Chen et al., 2018) developed by the authors' group. In NECP-X, the widely used 2D/1D method is adopted for the transport calculation, and the 2D transport calculation is performed using the method of characteristics (MOC). The MOC solver is used for the Dancoff correction factor calculation

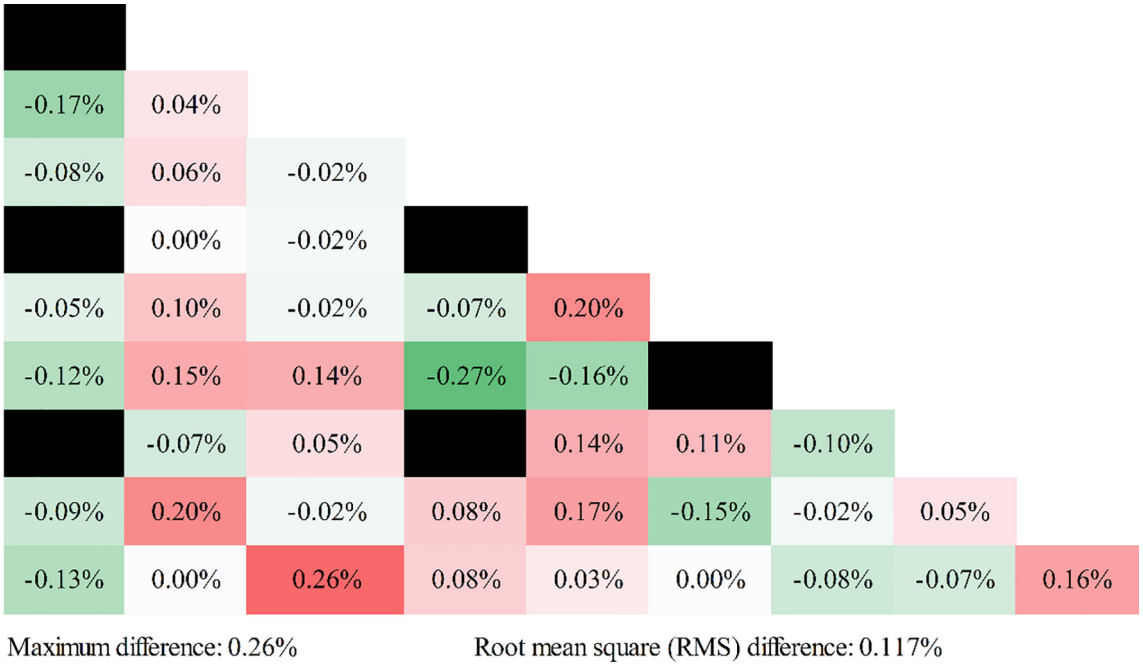

Fig. 11. Comparison of pin powers at 0 GWd/tU for VERA 2D benchmark.

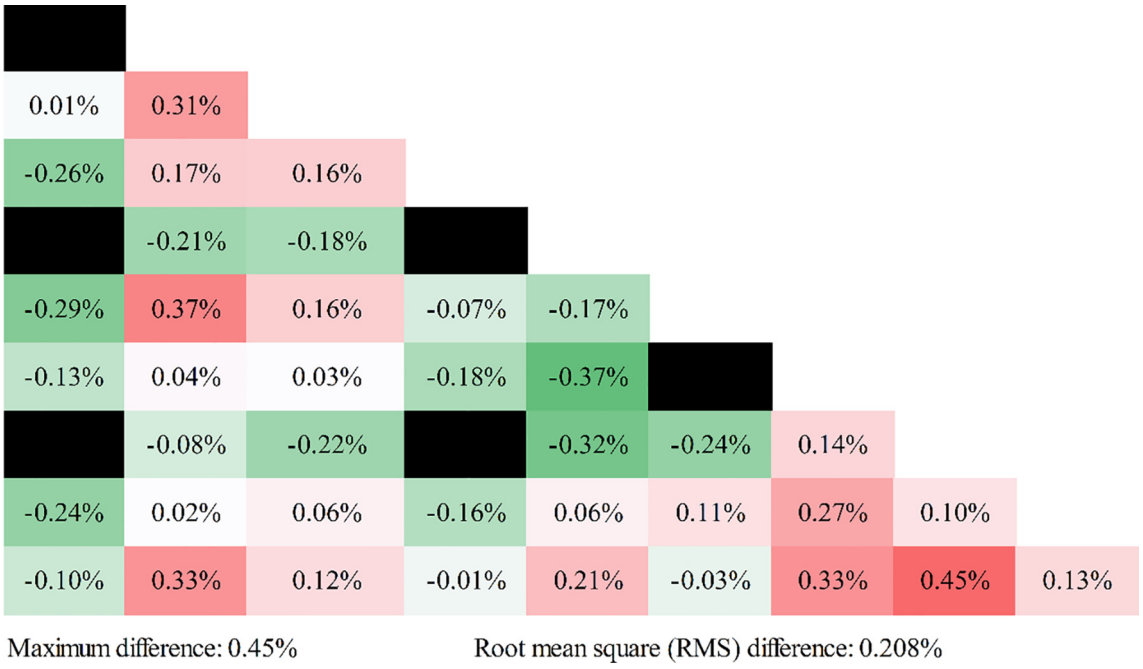

Fig. 12. Comparison of pin powers at 60 GWd/tU for VERA 2D benchmark.

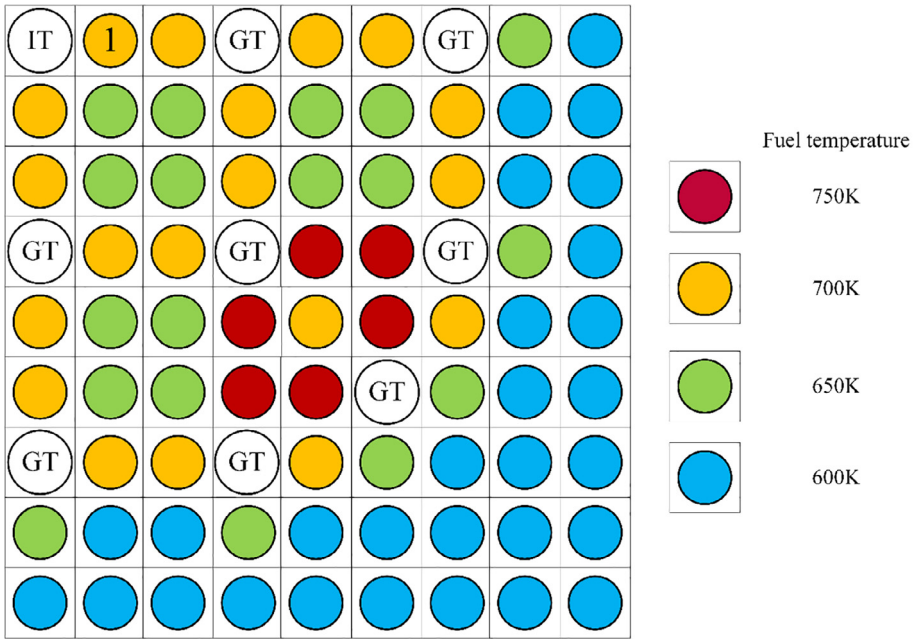

Fig. 13. Geometry of VERA 2C benchmark with temperature distribution.

Table 4
Infinite multiplication factor of VERA 2C benchmark with temperature distribution.

Reference k_{inf}	Calculated k_{inf}	Difference of k_{inf} (pcm)
1.18133 ± 0.00005	1.18272	139

in the present paper. The lethargy width of hyperfine group calculation is 0.00025. The ENDF/B-VII.0 is used for the hyperfine energy library and multi-group library generation.

3.1. 1-D pin cell problem

In this subsection, three different 1-D pin cell problems are calculated to analyze the computation time of the hyperfine group method in different situations. Firstly, the fuel temperature, material and configuration are set as VERA 1C benchmark. In this case, the fuel temperature and material composition in fuel rod are constant, nevertheless, the fuel rod is subdivided into 10 rings with equal volume to show the time to get spatially dependent cross sections. Secondly, the fuel rod is also divided into 10 rings as case

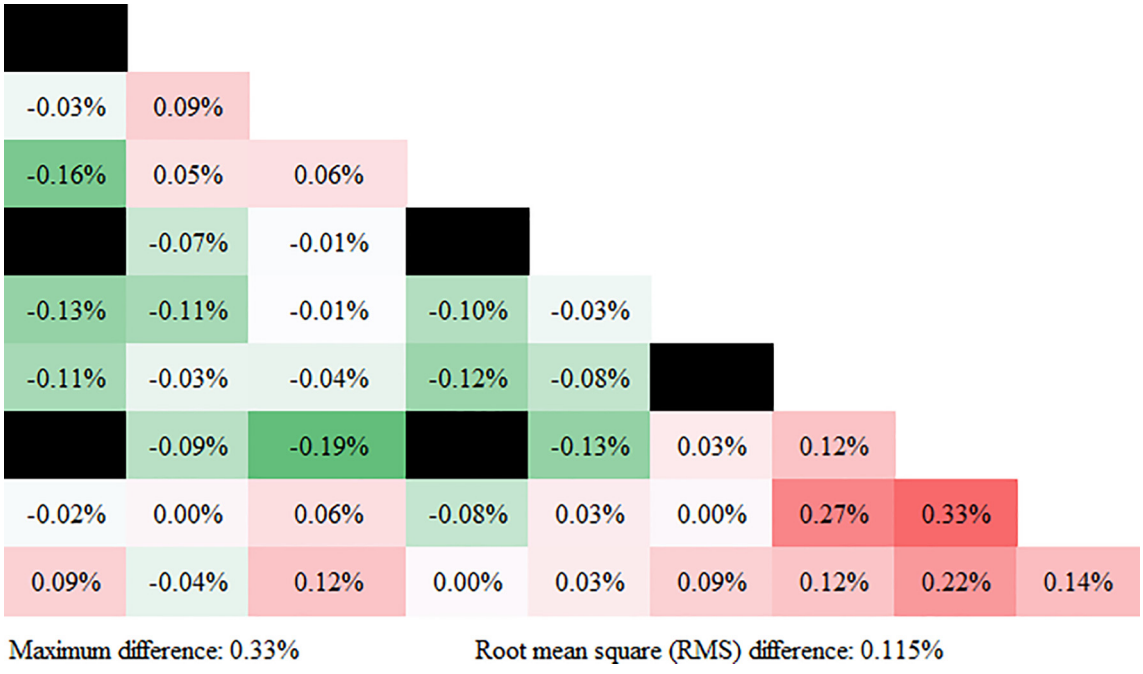

Fig. 14. Comparison of pin powers for VERA 2C benchmark with temperature distribution.

1, and the rings have different temperature. The temperature profile is shown in Table 1. In this case, the material composition in the fuel rod is constant. Thirdly, the 10 rings in the second case are set to have different material composition. The nuclides included in each ring comes from a burnt nuclear fuel. There are 287 nuclides in the fuel. And the fuel temperature uses an average value as the first case.

The calculation times for each case are given in Table 2. The Preprocess time given in the table is the time used by the procedures except the calculations of source term and collision probabilities, which includes reading the hyperfine group library, interpolating the hyperfine group cross sections versus the temperature and so on. In the first case, the total cross section is constant in the fuel rod, so that the collision probabilities can be calculated in advance and stored as the function of the total cross section. Therefore, the calculation time is the shortest, and it takes 0.38 s to get the spatially dependent cross sections. In the second case, the 10 rings are treated as different regions, so it takes more time to calculate the collision probabilities, and the time for the collision probabilities calculation is 4.4 s. In the third case, the there is a large number of nuclides in the fuel region, and it takes 7.11 s to calculate the source term. The above results indicate that if the hyperfine group method is directly used to the cases with radial temperature distribution, or with hundreds of fission products, the calculation time is unacceptable.

3.2. Lattice benchmark

In this subsection, several lattice problems from VERA benchmark (Godfrey, 2014) and VERA burnup benchmark (Kim, 2015) are tested to show the precision of the interpolation method proposed in this paper.

3.2.1. VERA 2C benchmark

The VERA 2C benchmark is firstly analyzed. The geometry of VERA 2C benchmark is shown in Fig. 5. In this benchmark, the fuel temperature is uniform in the assembly, at 900 K. The paper (Godfrey, 2014) provides the reference results of the infinite multiplication factor (k_{inf}) and pin power gotten by the Monte Carlo code KENO. The relative differences k_{inf} and pin power are respectively given in Table 3 and Fig. 6. The maximum difference and root mean square (RMS) difference of pin power are 0.18% and 0.095%, respectively. In order to show the accuracy of multi-group effective cross sections, a fuel pin denoted as pin 1 in Fig. 5 is analyzed. The reference results of the multi-group effective cross sections in this paper are obtained by a continuous energy Monte Carlo code. The statistical error of microscopic cross-sections obtained by the Monte Carlo code is less than 0.001%. The relative differences of multi-group effective absorption cross sections for U-238 and multi-group effective fission cross sections for U-235 in fuel pin 1 are shown in Fig. 7. For U-238, almost all the groups have small differences less than 1.0% and the maximum difference is 1.2%. For U-235, all the groups have small differences less than 0.9%. It can be confirmed from the above results obtained by the hyperfine group method with the interpolation method can accurately represent the multi-group microscopic cross sections of 2D lattice benchmark. The time of resonance calculation is 2.8 s. The problem is tested on Intel(R) Core(TM) i7-7700 CPU 3.6 GHz processor.

To verify that the proposed interpolation method can obtain correct spatially dependent cross sections within a fuel rod. The spatially dependent cross sections in VERA 2C benchmark are also calculated. The fuel rod is divided into 10 rings by equal volume. The relative differences of multi-group effective absorption cross sections for U-238 and multi-group effective fission cross sections for U-235 in fuel pin 1 are shown in Figs. 8 and 9, respectively. For U-238, almost all the groups have small differences less than 1.0% and the maximum difference is 1.6%. For U-235, all the groups have small differences less than 0.8%. It is obvious that the hyperfine group method with the interpolation method can accurately represent spatially dependent cross sections within a fuel rod.

3.2.2. VERA 2D benchmark with burnup

The VERA 2D benchmark is calculated to test performance of the proposed interpolation method when it is used to problems with burnup. The reference results of k_{inf} and pin power are from a Monte Carlo code coupling a burnup calculation code. The differences of k_{inf} versus burnup depth are shown in Fig. 10. The absolute value of the maximum difference of k_{inf} is about 140 pcm at 60 GWd/tU. The relative differences of one eighth assembly pin powers at 0 GWd/tU and 60 GWd/tU are shown in Figs. 11 and 12, respectively. For pin powers at 0 GWd/tU, the RMS difference and maximum difference are 0.117% and 0.26%. For pin powers at 60 GWd/tU, the RMS difference and maximum difference are 0.208% and 0.45%. The pin powers are close to the reference results.

The total time of resonance calculation in the VERA 2D burnup benchmark with 40 burnup steps is 496.8 s. The problem is tested on Intel(R) Core(TM) i7-7700 CPU 3.6 GHz processor.

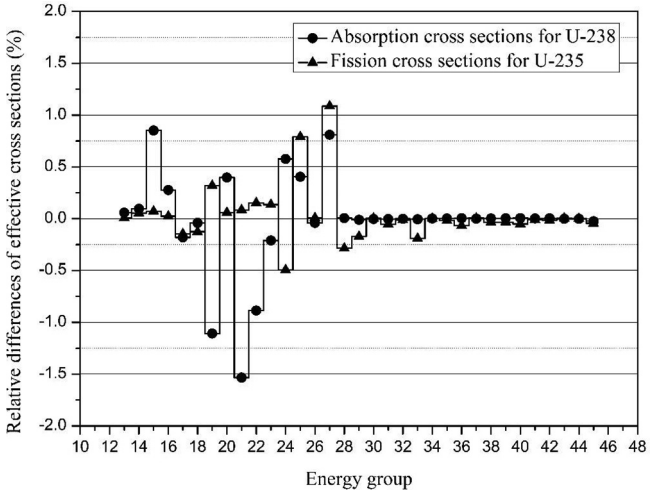

Fig. 15. Comparison of effective cross sections of fuel pin 1 in VERA 2C benchmark with temperature distribution.

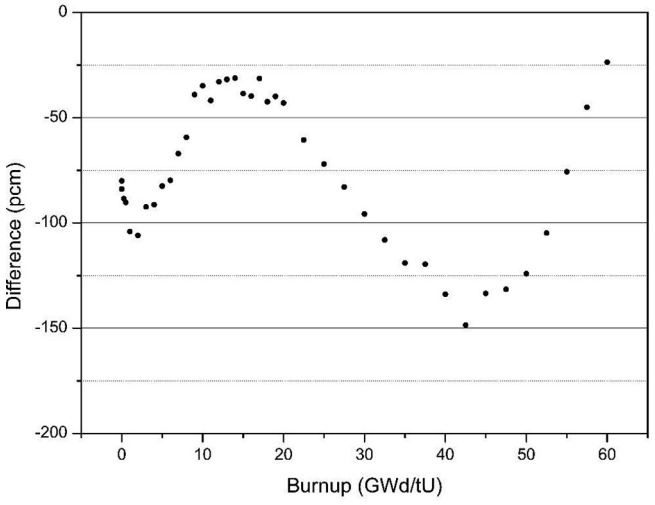

Fig. 16. Comparison of k_∞ vs burnup in lattice problem with burnup and different fuel temperature.

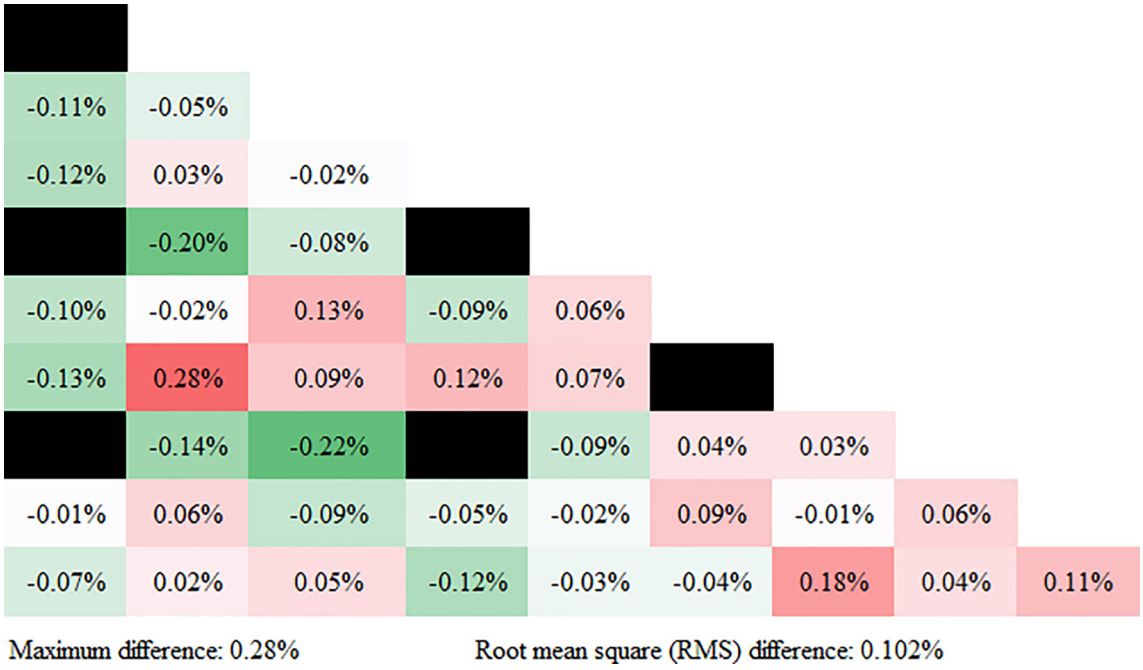

Fig. 17. Comparison of pin powers at 0 GWd/tU for lattice problem with burnup and different fuel temperature.

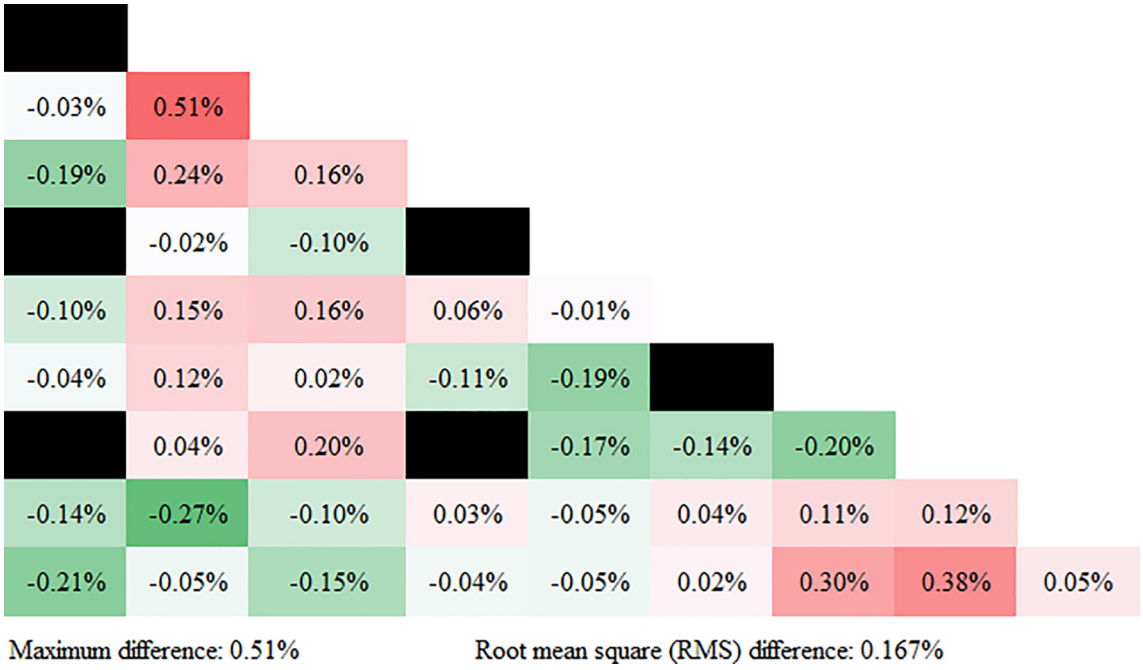

Fig. 18. Comparison of pin powers at 60 GWd/tU for lattice problem with burnup and different fuel temperature.

Table 5
Infinite multiplication factor and pin power of VERA 5A benchmark.

Reference k_{inf}	Calculated k_{inf}	Relative difference of k_{inf} (pcm)	Relative difference of pin power (%)	
			Max	RMS
1.00409 ± 0.00001	1.00507	98	1.78	0.57

3.2.3. Lattice with different fuel temperature

A problem is designed based on VERA 2C benchmark with temperature distribution to test the precision of the interpolation method when it is used to the case where the fuel temperature is different in a problem. The temperature distribution of the quarter assembly is shown in Fig. 13. The reference results are from the

continuous energy Monte Carlo code. Table 4 gives the results of k_{inf}. The relative differences of one eighth assembly pin powers are shown in Fig. 14. The maximum difference and root mean square (RMS) difference of pin power are 0.33% and 0.115%, respectively. A fuel pin signed as pin 1 in Fig. 13 is analyzed. The relative differences of multi-group effective absorption cross sections for U-238 and U-235 in fuel pin 1 are shown in Fig. 15. It can be confirmed from the results obtained by the hyperfine group method with the interpolation method reaches a good agreement with the reference results.

The problem is tested on Intel(R) Core(TM) i7-7700 CPU 3.6 GHz processor. The time of resonance calculation is 3.8 s.

3.3. Lattice with burnup and different fuel temperature

The burnup calculations are performed to the problem in the 3.2.3 section. The differences of k_{inf} versus burnup depth are shown in Fig. 16. The absolute value of the maximum difference of k_{inf} is 148 pcm at 42.5 GWd/tU. The difference of k_{inf} is waving in this test as shown in Fig. 16 and the reason is that the difference of k_{inf} is caused by two factors at the same time, resonance calculation method and interpolation. The relative differences of one eighth assembly pin powers at 0 GWd/tU and 60 GWd/tU are shown in Figs. 17 and 18, respectively. The pin powers are close to the reference results. For the pin powers at 0 GWd/tU, the RMS difference and maximum difference are 0.102% and 0.28%. For the pin powers at 60 GWd/tU, the RMS difference and maximum difference are 0.167% and 0.51%.

The total time of resonance calculation in this verification with 40 burnup steps is 1362.4 s. The problem is tested on Intel(R) Core (TM) i7-7700 CPU 3.6 GHz processor.

3.4. Whole-core benchmark

In order to prove the capability of the proposed method to treat the whole-core problem, a 2D whole-core benchmark, VERA 5A benchmark, is calculated and analyzed. The problem is tested on Intel(R) Xeon(R) CPU E5-2620 v3 CPU 2.40 GHz processor with 313 cores in parallel. The results of pin powers and k_{inf} are summarized in Table 5. The calculation time of VERA 5A benchmark is 5.9 s. Multi-level parallel method is implemented in NECP-X, including space, angular and ray parallel. The space parallel includes axial domain decomposition and radial region decomposition, which reduce the resonance calculation time greatly comparing with serial computing. It can be concluded that the hyperfine group method with the interpolation method has the ability of whole-core resonance calculation and the computation time is acceptable.

4. Conclusions

In this paper, some efforts have been made to apply the hyperfine group resonance calculation method to the practical lattice physics or direct whole-core neutronics simulation. An interpolation method is developed in the frame of the global-local self-shielding calculation method developed by the authors' group. In the global-local self-shielding calculation method, the equivalent 1-D cylindrical pin cells are established for the realistic pin cells in the analyzed system, and the equivalent 1-D cylindrical pin cells are independent on each other. Although the hyperfine group method can be applied to each 1-D pin cell, but it is impractical when the system is large, because there are many 1-D pin cells needing to be calculated. Therefore, a cross section interpolation method is developed to reduce the number of times that the hyperfine group method is performed when a large scale problem is analyzed. In this method, a series of typical equivalent 1-D cylindrical pin cells are established varying the Dancoff correction factor, burnup depth and fuel temperature, and the microscopic multi-group effective cross sections of the realistic pin cells are obtained by interpolation versus these three parameters.

The precision of the interpolation method is tested against several benchmarks including pin cell benchmark, lattice benchmark and whole-core benchmark. The numerical results show that the spatially dependent effective self-shielding cross sections, infinite multiplication factor and pin power obtained from the hyperfine group method with the interpolation method agree well with reference values from the Monte Carlo code. Moreover, the resonance calculation time is reduced significantly so that the hyperfine group method can be applied to the practical lattice and whole-core physics calculation.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.anucene.2019.107045.

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