A SUBGROUP METHOD BASED ON THE EQUIVALENT DANCOFF-FACTOR CELL TECHNIQUE COMPARED WITH THE FINE-STRUCTURE METHOD IN APOLLO3®

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ABSTRACT

We compare a newly implemented subgroup method, which is based on the equivalent Dancoff-factor cell technique, with the fine structure method in APOLLO3®. The new method obtains precise reaction rates and consequently is precise in predicting multiplication factor. It can reduce the time in the self-shielding calculation by a factor of 38 compared with the subgroup method based on the multi-cell approximation in a PWR Gd-UOX assembly calculation. The fine structure method obtains larger errors in reaction rates than the subgroup method, but the error compensation sometimes leads to small errors in multiplication factors. This work demonstrates the precision and the efficiency of the new method.

KEYWORDS: resonance self-shielding, subgroup method, SPH method, equivalent Dancoff-factor cell method, fine structure method

1. INTRODUCTION

Resonance self-shielding is a primary step in multigroup lattice calculations. The precision of the self-shielding method determines the precision of lattice calculations and subsequent core calculations. The fine-structure method (FSM) in APOLLO3® [1], has been developed based on the FSM of the APOLLO2 code [2]. The method performs the self-shielding calculations by solving the fine-structure equation.

The FSM combines the subgroup method with the equivalence theory, in order to use a coarse energy mesh and the mathematical probability tables that preserve the moments of point-wise cross sections. With the coarse group grid, the subgroup assumption that the cross sections are not correlated with the source term in a group, is not verified in the resolved resonance domain.

The remedy adopted by the FSM is the double equivalences: (1) The heterogeneous - homogeneous equivalence: the heterogeneous equation is first solved by using the subgroup method. We obtain

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the equivalent dilutions per region, per group and per resonant isotope by preserving the reaction rates. The reference reaction rates are then interpolated with the dilutions in the pre-tabulated reaction rates of infinite homogeneous media; (2) The multigroup equivalence: we calculate the self-shielded cross sections by iterations to preserve the reference reaction rates. The FSM obtains rather good precision, with a discrepancy of less than 300 pcm in multiplication factors in thermal reactor calculations. However it has difficulties to achieve a better precision.

The issue of the angular dependence of multigroup cross sections in resonance self-shielding was revealed recently [3]. The direct integration of the continuous-energy transport equation over an energy group results in a multigroup equation with angular-dependent total cross sections. Using the cross sections condensed by Monte Carlo scalar flux leads to an error around -200 pcm in the multiplication factor of a PWR UOX pin-cell [4]. The remedy is to apply the superhomogenization (SPH) method, which was originally introduced to preserve the reaction rates in spatial homogenization [5]. In the example above, the discrepancy in the multiplication factor could be reduced to less than 10 pcm, if we apply the SPH technique [4].

In the FSM, the multigroup equivalence, which is similar to the SPH, is performed. However, we still have -200 pcm to -300 pcm discrepancies in multiplication factors with the FSM. Both multigroup equivalence and SPH compute the cross sections by preserving the reference reaction rates. If the cross sections obtained by the multigroup equivalence can not reproduce the reference results, we believe that the reference reaction rates are not correct. In fact, in order to fix the slowing-down bias due to the use of a coarse energy mesh, the heterogeneous reaction rates are replaced by those of the infinite homogeneous media in the FSM. In consequence, the actual spatial reaction rates are lost in the heterogeneous-homogeneous equivalence.

To remedy this problem, we have developed a new subgroup method based on SPH technique (SG+SPH) [4] in APOLLO3. This method employs the LWR 383-group mesh, which is fine enough to avoid the heterogeneous-homogeneous equivalence. It employs the same Improved Direct Method (IDM) [1,4] of the FSM to solve the subgroup fine-structure equation. Then the SPH is carried out to obtain the cross sections that preserve the reaction rates. The IDM method is capable of treating resonant up-scattering and resonance interference, which are the two primary phenomena to be considered in the self-shielding calculations.

Our preliminary tests showed that the SG+SPH method was precise in the calculations of PWR cells and assemblies with UOX, MOX, and Gd-UOX fuels: the errors in multiplication factors are less than 50 pcm compared with the Monte Carlo references. However, the new method needs a long execution time in assembly calculations, due to the mixture treatment and the assembly collision probability calculation. When the number of mixtures increases, the number of self-shielding calculations increases proportionally, so does the number of calculations of assembly collision probabilities. In a depletion calculation of an eighth 17×17 fuel assembly, which has 45 pins of the same fuel material being divided into six rings, the number of mixtures can increase from one up to 270 as the burnup increases. Thus the number of the collision probability calculations with the multi-cell approximation (CP-MCA) at a burnup step can be up to 270 times the number at zero-burnup. Since the time for one assembly CP-MCA calculation is not trivial, this time increase becomes excessive for a practical calculation.

To remedy this issue, an Equivalent Dancoff Cell (EDC) method, originally proposed in [6], has

been recently implemented in APOLLO3 [7]. With the EDC method, we carry out only once the assembly CP-MCA calculation, by setting the fuel cross sections to 10^5 cm^{-1} and those of moderator and cladding to potential cross sections. Then the Dancoff factors of fuel pins are calculated using the assembly collision probabilities. For each fuel pin, an associated one-dimensional (1D) cylindrical cell, an EDC, is calculated to have the external radius determined by preserving the Dancoff factor in the two-dimensional (2D) geometry. Finally, the self-shielding calculation is only needed to be applied to the EDCs.

The preliminary tests showed that the EDC method gives similar results as the MCA method, the differences in multiplication factor of the two methods are generally less than 15 pcm. However, the EDC method can reduce the self-shielding time of an assembly by a factor of 16 to 53 compared with the MCA method [7]. In this paper, we will compare the calculations of fuel cells and assemblies by the EDC method and the FSM. Section 2 presents a brief resume of the theory of the EDC-based SG+SPH method. Section 3 gives numerical results. The conclusions are given in the end.

2. THEORY

The SG+SPH method was presented in detail in our paper [4] and the EDC method implemented in APOLLO3 was described in Ref. [7]. Here we give a brief review of the theory.

2.1. The Subgroup Method Based on the Fine-Structure Equation and the SPH

In the neutron slowing-down domain around the resonance energy, it is supposed that there is no fission and the neutron-nucleus scattering is primarily elastic scattering. Therefore, the neutron source in a region i can be defined as

$$R_{0i}\Phi_i(u) + R_{1i}\Phi_i(u), \tag{1}$$

where R is the scattering operator and the indexes 0 and 1 stand for resonant and moderator isotopes, respectively. By factorizing the flux into a product of a constant macroscopic flux $\chi_i(u) = \chi(u)$ and a local fine-structure factor $\phi_i(u)$, $\Phi_i(u) = \chi_i(u)\phi_i(u)$, and applying the fine-structure assumption [8], we obtain the collision-probability based fine-structure equation,

$$\Sigma_i(u)V_i\phi_i(u) = \sum_j P_{ij}(u)V_j\left[N_{0j}r_{0j}\phi_j(u) + \Sigma_{s1j}(u)\right], \tag{2}$$

where $r_{0i} = R_{0i}/N_{0i}$ and N_0 is the number density of the resonant isotope.

The subgroup method is assumed to apply to a fine energy grid. Using the "Toutes Résonances" (TR) approximation [8], we have

$$(r_0\phi)_g \approx (r_0\phi)_g^{TR} = \sum_{g'}(r_0\phi)^{g'\to g}, \tag{3}$$

where $(r_0\phi)^{g'\to g} = \sum_x a_x p_x^{g'\to g}\tau_{s0x,g'}$, and the resonant scattering rate $\tau_{s0x,g} = \dfrac{1}{\Delta u^g}\int_g du\sigma_{s0x}(u)\phi(u)$. $a_x = N_{0x}/N_0$ is the number density proportion of resonant isotope x in the mixture, $p^{g'\to g}$ is the probability for a neutron to scatter from group g' to group g after the collision.

The mathematical probability tables [8] are employed to compute the group-averaged quantities. For a mixture containing X resonant isotopes, the probability table is

$$\{p_k, \sigma_{t,k}, \sigma_{\rho x,k},\ k = 1, \ldots, K,\ x = 1, \ldots, X\}\,, \tag{4}$$

where p, σ_t and $\sigma_{\rho x}$ are the probability, the total cross section and the partial cross section for reaction ρ and isotope x, respectively. K is the order of the probability table.

Finally, the fine-structure-assumption based equation is written for a subgroup k in group g as

$$\left[\Sigma_{t1i} + N_{0i}\sigma_{t,k}\right] V_i \phi_{i,k} = \sum_j P_{ij,k} V_j \left[N_{0j} \sum_x a_x p_x^{g\to g} \sum_{l=1}^{K} p_l \sigma_{s0x,l} \phi_{j,l} + N_{0j} \sum_{g'\neq g} (r_0\phi)_j^{g'\to g} + \Sigma_{s1j} \right]. \tag{5}$$

The Improved Direct Method (IDM) [1,4] is employed to solve Eq. (5). We obtain the region-wise group-averaged flux and reaction rates. By using the mixture probability tables and the TR model, the IDM is capable to solve Eq. (5) with consideration of resonance interference and resonance up-scattering.

Due to the angular dependence issue of multigroup cross sections, the cross sections condensed by the scalar flux can not reproduce the reference results. In consequence, the SPH was applied to the subgroup solution to obtain the multigroup cross sections that preserve the subgroup reaction rates. The detail presentation of the SPH is given in Ref. [4].

2.2. The Equivalent Dancoff-Factor Cell Method

As presented in the paper [4], the SG+SPH method gives results in good agreement with Monte Carlo references. However, due to the employment of the mixture treatment and the collision probability calculations using the MCA approximation, the running time can become prohibitive for an assembly depletion calculation.

The Equivalent Dancoff-factor Cell (EDC) method [6] transforms a 2D geometry into a set of 1D cylindrical cells by preserving the 2D Dancoff factors, the EDCs, and carries out self-shielding calculations only on the EDCs. Since the collision probability calculations of 1D cylindrical cells are much faster than those of a 2D geometry, we can expect a drastic reduction in the CPU time of the self-shielding calculation.

The EDC method in APOLLO3 employs the collision probabilities to determine the EDCs. In the Dancoff factor calculations, the fuel cross sections are set to a large value, 10^5 cm^{-1}, and those of the moderator and the cladding are set to the potential scattering sections.

Suppose that a 2D lattice system has a set of fuel pins, $F_l, l = 1, L$. The Dancoff factor for pin F_l is defined as

$$D_{F_l}^{2D} = \frac{P_{esc,F_l}^{2D}}{P_{esc,F_l}^{isol}} = \frac{1 - P_{F\leftarrow F_l}^{2D}}{1 - P_{F_l\leftarrow F_l}^{isol}}. \tag{6}$$

where P_{esc,F_l} is the fuel escape probability of pin F_l defined as the probability that a neutron born uniformly in the fuel pin makes its first collision in moderator or cladding. The index $2D$ stands

for the 2D lattice system and the index $isol$ stands for the situation in which an isolated fuel pin is surrounded by an infinite homogeneous moderator medium. $F = \sum_{l=1}^{L} F_l$, stands for the set of fuel pins in the geometry. The 2D collision probabilities are computed using the CP-MCA option.

To each fuel pin F_l, we associate a 1D cylindrical isotropically-reflected cell with the same pin with an external moderator radius R_l. Its Dancoff factor is defined as

$$D_{F_l}^{1D}(R_l) = \frac{P_{esc,F_l}^{1D}(R_l)}{P_{esc,F_l}^{isol}} = \frac{1 - P_{F_l \leftarrow F_l}^{1D}(R_l)}{1 - P_{F_l \leftarrow F_l}^{isol}}, \tag{7}$$

using the 1D cylindrical collision probability calculations with the same cross sections employed in the 2D calculation. To obtain the 1D cylindrical pin that preserves the Dancoff factor in the 2D geometry, from Eqs. (6)(7), we only need to solve the equation

$$P_{F_l \leftarrow F_l}^{1D}(R_l) = P_{F \leftarrow F_l}^{2D}. \tag{8}$$

The solution is obtained by a binary search. The 1D EDCs need to be calculated once and for all. The self-shielding calculations are applied to these EDCs.

3. NUMERICAL RESULTS

We compare the self-shielding methods, the MCA-based and EDC-based SG+SPH methods and the FSM, in PWR fuel cell and fuel assembly calculations. The APOLLO3 flux calculations were carried out by the 2D TDT method of characteristics (MOC) solver. The anisotropic order was set to P_3 when using the SG+SPH methods, and it was set to P_3 or P_0 with transport correction (P_0c) when using the FSM. The subgroup methods employed the LWR 383-group energy mesh and the mixture treatment; the self-shielding was applied to groups 43 to 351, covering the energy domain from 111.535 keV to 0.55549 eV. The FSM options employed the SHEM 281-group energy mesh and the mixture treatment; the self-shielding was applied to groups 43 to 93, covering the energy domain from 49.9159 keV to 22.5243 eV, which is the recommended self-shielding range for using the FSM.

Using the TR scattering model, both the SG+SPH method and the FSM are capable to take into account the resonant up-scattering. Our preliminary tests showed equivalent precision in calculations with or without the consideration of up-scattering. Due to the paper length limit, only the results without considering the up-scattering are given in the following. In consequence, the reference TRIPOLI-4 Monte Carlo calculations employed the traditional SVT (Sampling of the velocity of the target nucleus) model [9]. The TRIPOLI-4 and APOLLO3 calculations were carried out using the CEA V514 library, which is based on JEFF-3.1.1 nuclear data evaluation [10].

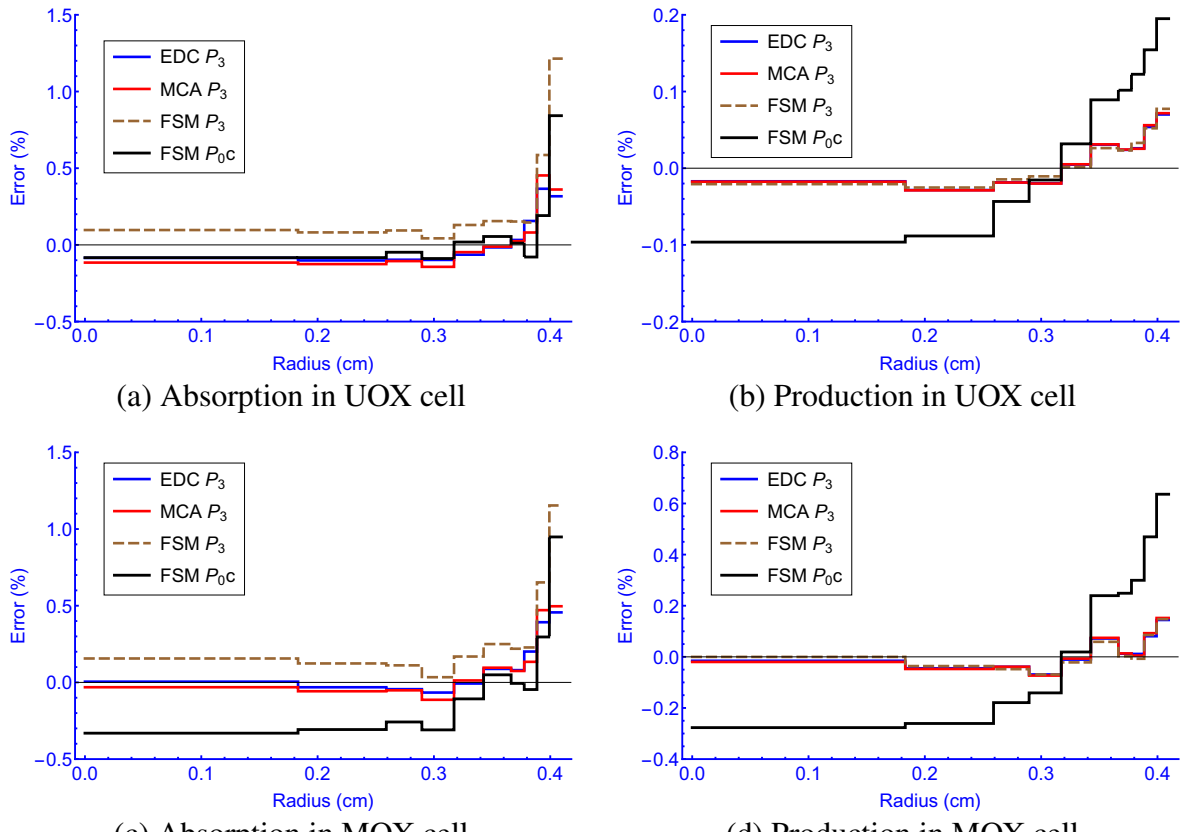
3.1. PWR Fuel Cell Calculations

Two typical PWR UOX and MOX cells were selected for the preliminary tests. The geometry and material compositions of the two cells are defined in Ref. [4]. For self-shielding calculations, the fuel pin was subdivided into 10 rings, corresponding to 20%, 20%, 10%, 10%, 10%, 10%, 5%, 5%, 5%, 5% of the fuel volume, respectively. For flux calculations, each of the 10 fuel rings was further subdivided into eight sectors.

Table 1 shows the k_{eff} discrepancies in both UOX and MOX cell calculations. The MCA and EDC methods have obtained similar results, the k_{eff} errors are less than 80 pcm compared with the references. The FSM P_3 option underestimates the k_{eff} up to -280 pcm. The FSM P_0c option predicts rather well the k_{eff} value.

Table 1: PWR fuel cell k_{eff} discrepancies

	UOX cell		MOX cell	
Option	k_{eff}	Δk_{eff} (pcm)	k_{eff}	Δk_{eff} (pcm)
MCA P_3	1.26950	36	1.09551	-66
EDC P_3	1.26940	26	1.09543	-74
FSM P_3	1.26683	-231	1.09337	-280
FSM P_0c	1.26855	-59	1.09662	45
TRIPOLI-4	1.26914 $\pm$ 5 pcm		1.09617 $\pm$ 5 pcm	



(a) Absorption in UOX cell

(b) Production in UOX cell

(c) Absorption in MOX cell

(d) Production in MOX cell

Figure 1: The per-ring reaction rate errors in fuel cells

Fig. 1 gives the spatial discrepancies in the reaction rates. The MCA and EDC options of the SG+SPH method result in a slight underestimation in the inner rings and a slight overestimation in the outer rings. The errors are less than 0.5% in absorption rates and less than 0.1% in production rates. This explains why the MCA and EDC methods predicts well the multiplication factors.

The FSM P_3 option overestimates the absorption in all rings, whereas it estimates well the production. Therefore, the multiplication factors are underestimated. With the FSM P_0c option, the underestimation in inner rings and the overestimation in outer rings are worsened in both absorption and production. However, the errors in absorption and production are compensated and the multiplication factors are in better agreement with the references compared with the FSM P_3 option.

3.2. PWR Fuel Assembly Calculation

We chose to calculate the PWR UO_2 assembly defined in the LWR benchmark problem suit [11]. Since it has five Gd-bearing UO_2 cells, it is named "Gd-UOX assembly" hereafter. The calculations were carried out at burnup 0 with hot and 0% void fraction conditions. To avoid the interpolation of nuclear data in both TRIPOLI-4 and APOLLO3 calculations, the temperatures were set to 974 K for fuel and 574 K for structural material and moderator. The calculations were carried out on the eighth assembly. In the self-shielding calculations, the fuel pins were subdivided into 10 rings using the same dividing scheme employed in Section 3.1. In the flux calculations, each of the 10 rings was further subdivided into eight sectors. The calculations were carried out by using the CEA V514 library based on JEFF-3.1 nuclear data evaluation [10].

Only the FSM P_0c option presents large error in k_{eff} (Table 2), while the three others agree well with the reference. Figs. 2 and 3 presents the errors in spatial absorption and production rates, where the omitted results of the MCA method are similar to those of the EDC method. The results of the EDC and MCA methods agree well to the references, with maximum errors of 0.26% in absorption rates and 0.35% in production rates.

With the FSM P_3 option, both absorption and production rates are underestimated in the Gd-UOX cells and overestimated in the UOX cells. The good agreement in k_{eff} is obtained by error compensation. With the FSM P_0c option, the underestimation in the Gd-UOX cells is worsened, while the overestimation in the UOX cells is reduced, compared with those of the FSM P_3 option. The errors in absorption and production are not completely canceled out and they result in a larger k_{eff} error.

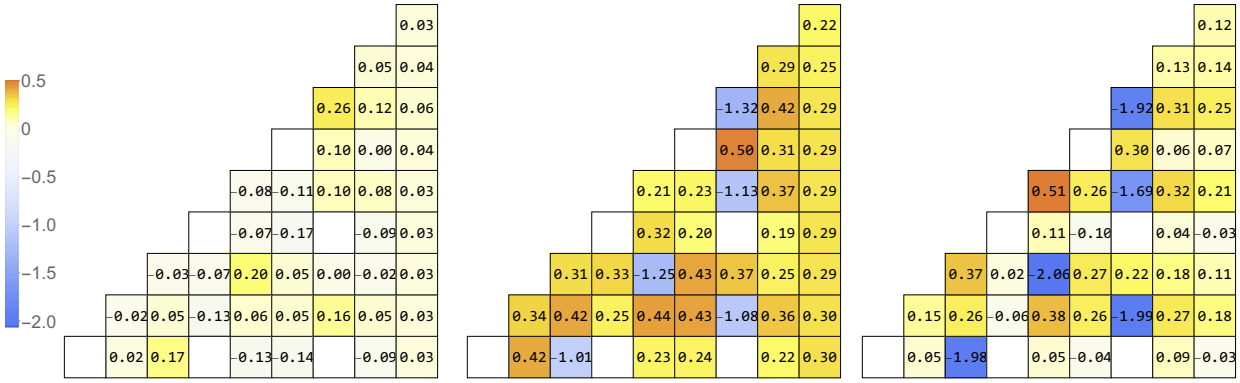
Table 2 also gives the CPU times in self-shielding calculations. The EDC method reduces the CPU time by a factor of 38 compared with the MCA method, while keeping similar precision in k_{eff} and reaction rates. This fact demonstrates the precision and efficiency of the EDC method.

4. CONCLUSIONS

We have compared the newly developed EDC-based SG+SPH method with the FSM method in the PWR fuel cell and assembly calculations. The results show that both EDC-based and MCA-based SG+SPH methods are precise in reaction rates and therefore precise in multiplication factors. The

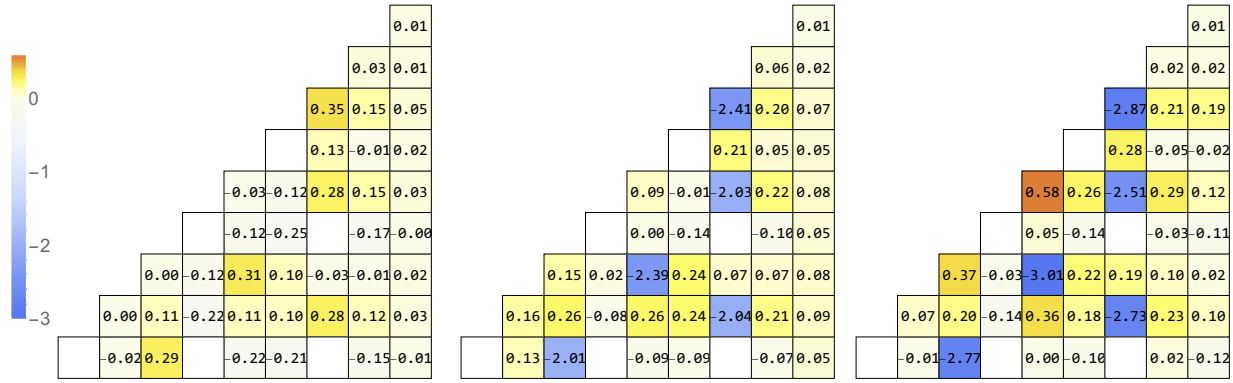
Table 2: PWR Gd-UOX assembly k_{eff} discrepancies and CPU times

Option	k_{eff}	Δk_{eff} (pcm)	Mixture-PT (s)	Self-Shield (s)
MCA P_3	1.12961	-51	27	798
EDC P_3	1.12978	-34	29	21
FSM P_3	1.13018	6	34	92
FSM P_0c	1.13322	310	35	91
TRIPOLI-4	1.13012 $\pm$ 2 pcm			



(a) EDC P_3 (b) FSM P_3 (c) FSM P_0c

Figure 2: The pin-wise absorption rate percent errors in the Gd-UOX assembly



(a) EDC P_3 (b) FSM P_3 (c) FSM P_0c

Figure 3: The pin-wise production rate percent errors in the Gd-UOX assembly

EDC method is much more efficient than the MCA method by reducing the CPU time by a factor

of 38 in the Gd-UOX assembly calculation.

With the FSM P_3 or P_0c options, we obtained larger discrepancies in absorption or production rates than with the SG+SPH methods. This proves that the spatial reaction rates are not preserved by the FSM. Sometimes we may obtain a multiplication factor in good agreement with the reference, however it is due to the error compensation.

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