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A Correction Ratio Incorporating Burnup for Combined Fission Matrix Theory

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1. Introduction

The Monte Carlo method has been widely used in neutronics-burnup coupled calculation due to its high fidelity with the capability to simulate exact geometry and a continuous energy spectrum. During criticality calculation, the Monte Carlo method simulates multiple batches of neutrons. The first-generation fission neutrons generated in each batch are employed as the initial neutrons for subsequent simulation batches. To attain an acceptable level of accuracy, a reasonable count of inactive cycles is necessary to converge towards the true source distribution, after which the desired parameters are evaluated through subsequent active batches.

However, researches[1][2] indicate that the Monte Carlo method encounters challenges in achieving convergence for the fission rate distribution in a loosely-coupled system, such as a large reactor core. Computation of burnup problems using the Monte Carlo method demands several criticality calculations, and a single criticality calculation can be time-consuming, thus warranting the adoption of a swifter approach. The combined fission matrix method proves highly efficient in expediting these calculations and has been partially developed in previous studies[3]. In this paper, we develop a burnup correction ratio to compensate for the errors induced by heterogenous burnup distribution to the combined fission matrix method.

The fission matrix method was first used to accelerate Monte Carlo algorithms[4]. Recently, it has become more popular due to its advantages in fast convergence and accuracy. The hallmark of the combined fission matrix is its utilization of databases obtained through fast fixed-source computations, where fixed-source is an efficient computational method. This approach circumvents the time-consuming criticality calculations, enabling swift attainment of criticality results. The principles of the combined fission matrix have found practical utility in diverse neutronics computations, encompassing tasks such as complete core assessments[5], simulations of spent fuel pools[6], and dynamic simulations involving conceptual reactors[7].

In this paper, the application of the combined fission matrix method theory to fuel depletion computation is developed. Additionally, a novel correction ratio theory is put forth to mitigate the error caused by fuel burnup. An exploration of fission rate distribution and eigenvalues is conducted within a compact 5*5-assembly core model, compared to a Monte Carlo reference calculation.

2. Methods

This section outlines the technical approaches employed to enhance precision while optimizing computational efficiency. This encompasses the elucidation of matrix combination principles as well as the establishment of correction ratio.

2.1 Combined Fission Matrix Theory

The foundation of the combined fission matrix (CFM) theory lies in the fission matrix theory, which represents an acceleration method for Monte Carlo criticality calculations in its initial stages of development. Sean Carney has presented a mathematically rigorous proof[8] demonstrating that an eigenvalue problem can be formulated using the expression depicted in Eq. (1):

$$S_I = \frac{1}{K}\sum_{j=1}^{N} F_{I,J} S_J \qquad (1)$$

When a physical model is partitioned into multiple regions, each element in the fission matrix F represents the fission neutrons produced in the I region due to the fission neutrons originating in the J region. The principal eigenvalue of this matrix mirrors the system eigenvalue formally, and the principal eigenvector offers insight into the fission neutron source distribution for this particular predicament. Equation (2) can likewise be expressed in the format of a matrix-vector relationship:

$$\vec{S} = \frac{1}{K}\overline{F}\vec{S} \qquad (2)$$

The vector S here, with a length of N corresponding to the total number of regions, denotes the distribution of newly generated fission neutrons for a single generation across these all regions. The symbol K maintains equivalence with the formal eigenvalue k_{eff}, characterizing the criticality of this problem. Therefore, the criticality eigenvalue problem has been transformed into finding the $N \times N$ full fission matrix F.

In practical scenarios, Monte Carlo simulations often employ a finely detailed mesh, leading to the generation of a huge fission matrix. Obviously, recalculating the complete fission matrix for each alteration in the system becomes impractical. To address this, the combined fission matrix technique has been introduced.

This approach combines fission matrices derived under diverse conditions, generating a novel fission matrix for assessing heterogeneous systems. As a result, a new fission matrix is constructed without the need for iterative Monte Carlo computations during condition

modifications. These conditions include factors such as assembly types, fuel temperature, or burnup.

In the process of combination, a straightforward presumption is made, postulating that the count of fission neutrons generated in cell *i* per source neutron from cell *j*, denoted by the fission matrix element F_{ij}, is exclusively depend upon the material characteristics of the recipient cell *i*. To illustrate, consider a model incorporating two distinct materials, M_1 and M_2, depicted in Fig. 1.

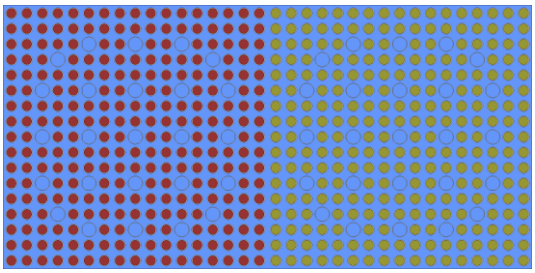
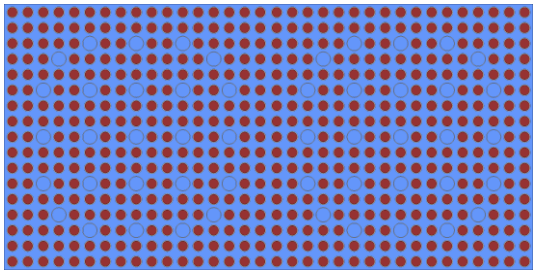


Fig. 1. Two-assembly model consists of two distinct materials

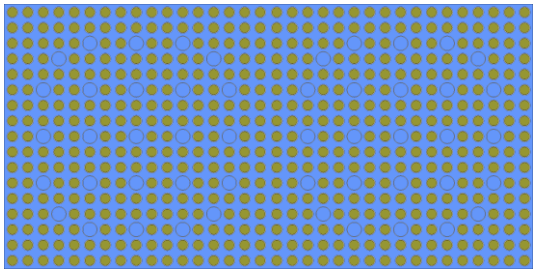
Termed as F^{M_1} and F^{M_2}, the fission matrices for these two materials are established, while F represents the combined fission matrix encompassing the entire system. Thus, the relationship for F can be expressed as detailed in Equation (3).

$$F_{ij} = \begin{cases} F_{ij}^{M_1}, \text{if cell } i \text{ is occupied by M1} \\ F_{ij}^{M_2}, \text{if cell } i \text{ is occupied by M2} \end{cases} \quad (3)$$

where the F^{M_1} and F^{M_2} are calculated by fixed source simulation using homogeneous model filled with material M_1 or M_2 shown in Fig. 2(a) and (b).



(a) homogeneous model consisting only of material M_1



(b) homogeneous model consisting only of material M_2

Fig. 2 . Homogeneous model used to calculate the fission matrix

2.2 Correction Ratio Theory

An essential point of consideration pertains to the disregard of differentiations between the source cell and the destination cell within this combination methodology. It should be acknowledged that moderation and absorption transpiring within intermediate cells could indeed exert an impact on the neutron spectrum observed in the ultimate destination cell. However, the postulation attributing the determination of flux at the destination to localized moderation and absorption characteristics still stands as a general assumption. This is underscored by the fact that fission events within the target cell predominantly arise from thermal neutrons. Given the limited transport capability of thermal neutrons and their substantial local absorption, the characteristics of the target cell significantly govern the thermal flux in that region. Consequently, it is rational to deduce that information pertaining to the target cell itself adequately facilitates a reasonable estimation of its fission rate.

Nonetheless, the new matrix F still has errors in estimating the true matrix between two regions with different properties. This discrepancy arises due to the evident influence exerted by neighboring assemblies on the neutron spectrum at the boundary. Rectifying this boundary discrepancy necessitates the application of correction ratios. If we denote the genuine fission matrix for the system as F, the corrective matrix can be defined in accordance with Equation(4).

$$F \cdot \vec{S} = C \cdot F \cdot \vec{S} = K \cdot \vec{S} \quad (4)$$

Assume the correction matrix C is a diagonal matrix, then Eq.(4) can be written as:

$$\begin{pmatrix} c_1 & & & & \\ & c_2 & & & \\ & & \ldots & & \\ & & & c_{n-1} & \\ & & & & c_n \end{pmatrix} \cdot F \cdot \vec{S} = F \cdot \vec{S} \quad (5)$$

then

$$c_i = \frac{FS_i}{FS_i} \quad (6)$$

Obviously, Eq.(6) incorporates the unknow authentic fission matrix F, thus mandating the estimation of the correction matrix C. In the context of this study, the precise correction ratios are defined as follows:

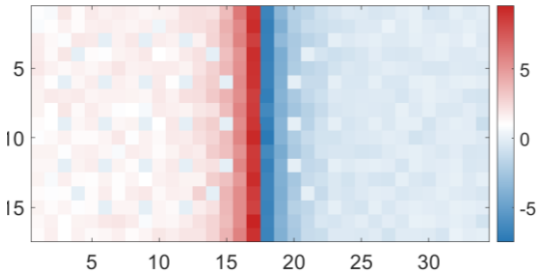
$$r_i = \frac{fr_i \text{ (real model)}}{fr_i \text{ (homogeneous model)}} \quad (7)$$

where the *fr* represents fission production in the specific model. Then the estimated matrix after corrected can be calculated by Eq.(8).

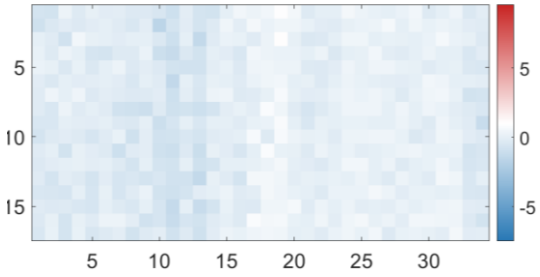
$$F^* \cdot \vec{S} = \begin{pmatrix} r_1 & & & & \\ & r_2 & & & \\ & & \ldots & & \\ & & & r_{n-1} & \\ & & & & r_n \end{pmatrix} F \cdot \vec{S} \qquad (8)$$

As an illustrative example, consider the configuration represented in Fig. 1. The correction ratio for the left assembly is found by dividing the fission production calculated from the real model by the one obtained using the setup in Fig. 2(a). Similarly, the correction ratio corresponding to the right assembly is established by dividing the actual model's fission production by that of the homogeneous model depicted in Fig. 2(b). These correction ratios constitute the diagonal elements of the correction matrix *C*. It is important to note that the fission production in this context is ascertained through Monte Carlo uniform fixed-source simulations.

The material enrichment for the left assembly is 1.6%, whereas the right assembly possesses an enrichment of 2.4%. The fundamental mode eigenvector error associated with the uncorrected directly combined fission matrix is illustrated in Fig. 3(a), while Fig. 3(b) displays the error in the corrected fission neutron source distribution. Application of the correction ratio results in a reduction of the root-mean-square error in the relative source distribution from an initial value of 2.6% to a final value of 0.4%.



(a) relative error before correction(%)



(b) relative error after correction(%)

Fig. 3. Relative error of the fission neutron source distribution before and after correction ratio applied.

The fuel utilized within the aforementioned model is characterized as fresh fuel. However, in the burnup computation, one of the pertinent considerations for the correction ratio is the combustion depth. Concerning the two-component model illustrated in Fig. 1, a scenario is examined where the burnup of the left assembly remains unchanged, while the burnup of the right assembly is varied. For instance, in Fig. 4, a specific instance is presented involving the foremost row of fuel rods within the geometric model. In this scenario, the correction ratio for the No.17 fuel pin, situated at the intersection of the two components, is calculated. The outcomes of this calculation are portrayed in Fig. 5, elucidating the behavior of the material correction ratio, which exhibits commendable parallelism. Notably, this correction ratio incorporates considerations of both enrichment and burnup.

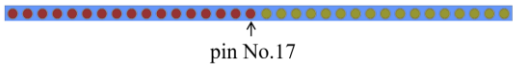


Fig. 4. Correction ratio curve calculation model.

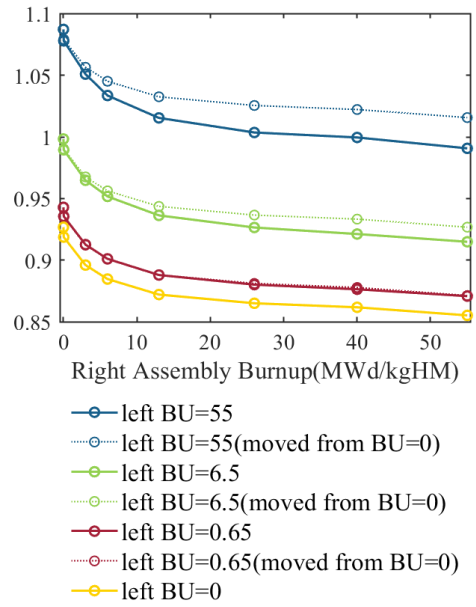


Fig. 5. Parallelism of material correction ratio curves

However, it is evident that the curve resulting from a direct translation does not perfectly align with the curve derived from direct calculations. Denoting the authentic burnup-enrichment composite correction ratio, named as material correct ratio, for each burnup step as r^i_{true}, and the correction ratio obtained through panning as r^i_{para}, a re-correction factor $h(i)$ is hypothesized to exist exclusively linked to the burnup of the right assembly. This re-correction factor adheres to the subsequent equation:

$$r^i_{para} \times h(i) = r^i_{true} \qquad (9)$$

$$h(i) = \frac{r^i_{true}}{r^i_{para}} \qquad (10)$$

The graphical representation of $h(i)$ in relation to the burnup of the right assembly is depicted in Figure 5. Employing the final combustion step data as the axis of

symmetry, a distinct cubic curve can be cohesively established with the known data derived from the fresh right assembly. This enables the independent determination of $h(i) = h(b) = m_1 b^3 + m_2 b^2 + m_3 b + m_4$, where m signifies the coefficient and b signifies the burnup of the right assembly.

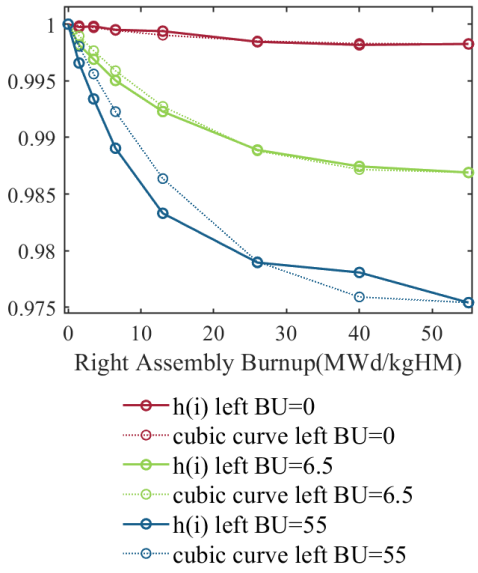


Fig. 6. Change of re-correction factor $h(i)$ with burnup of the right assembly and the cubic function fitting.

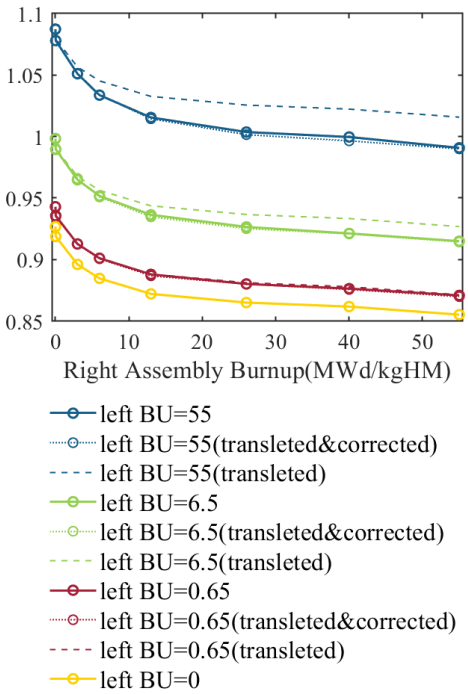


Fig. 7. Comparison of true correction ratios with material correction ratios after translation and re-correction.

The utilization of the cubic curve re-corrections within the translation methodology, as demonstrated in Fig. 5, yields the outcomes displayed in Fig. 7. The translated and re-corrected material correction ratios exhibit a nearly coincident alignment with the curves denoting directly computed correction ratios. This practice contributes to efficiency by economizing the time required for computing correction ratios across the entire spectrum of fuel burnup permutations.

While the aforementioned considerations are tailored to the juxtaposition of two components on the left and right, the inherent geometric symmetry underscores the applicability of a similar computational approach between assemblies situated at the top and bottom, as well as those diagonally contiguous.

In synthesis, the quest for the correction proportion stemming from one fuel, denoted as M_1, in relation to an adjacent material, represented as M_2, necessitates the computation of the following three curves:

(1) With the burnup of M_1 assembly set at 0, assess the material correction ratio across diverse burnups of M_2 assembly.
(2) Keeping the burnup of M_2 assembly at 0, investigate the material correction ratio across varying burnups of M_1 assembly.
(3) Maintaining the burnup of M_2 assembly at the maximum value within the database, explore the material correction ratio across diverse burnups of M_1 assembly.

2.3 CFM database

Clear from the earlier discussion, the database within the framework of the CFM method is divided into two parts, encompassing a fission matrix database alongside a correction ratio database. The procedure for constructing the fission matrix database is outlined in Fig. 8.

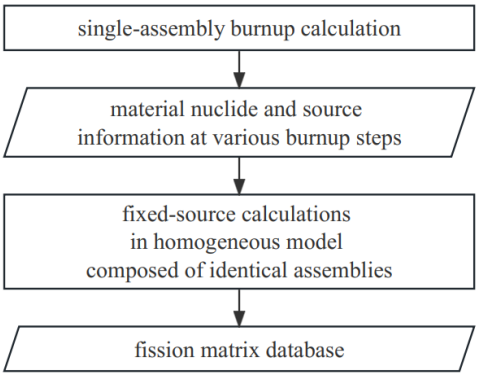


Fig. 8. Calculation procedure of fission matrix database.

In the initial stage, critical burnup calculation for an individual assembly is undertaken. This phase uses a basic model without accounting for factors like control rods, while using a fully reflective boundary condition. Within the small single-assembly model, conventional Monte Carlo simulations ensure efficient computations, sparing significant time consumption. During this stage,

the aim is to obtain nuclear isotope and source distribution information for each burnup step.

In the next phase, the utilization of the fission matrix definition facilitates the computation of its values. It is established that F_{ij} represents the neutrons engendered within region i due to the influence emanating from region j. Thus, a single fission matrix column is obtained by applying a fixed source to a defined area, like a designated fuel pin, to initiate a fixed-source calculation. The application of geometric symmetry in this context serves to streamline the process of fixed-source calculation, effectively circumventing the requirement to individually traverse each distinct fuel rod.

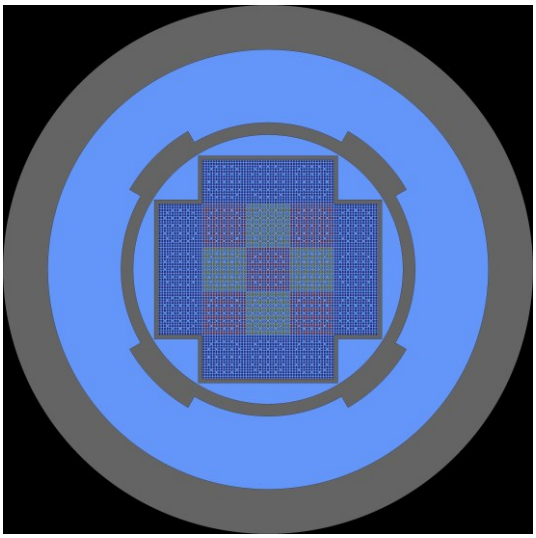
The computation approach for the material correction ratio database has been presented in the concluding segment of Section 2.2 and will not be reiterated within this context. Performing fixed-source calculations for correction ratios also requires access to material nuclide data at different burnup steps. Therefore, the calculation of single-assembly burnup stands as a prevalent preliminary stage requisite for both the fission matrix database and the correction ratio database.

Currently, the speed of preparing the database is not particularly fast. Nonetheless, upon the completion of the database, subsequent burnup calculations for reactor cores will be notably expedited. Furthermore, adjustments to core configurations will no longer necessitate the repeated construction of the database. Enhancing the efficiency and accuracy of the database calculation process stands as a prospective direction for future endeavors.

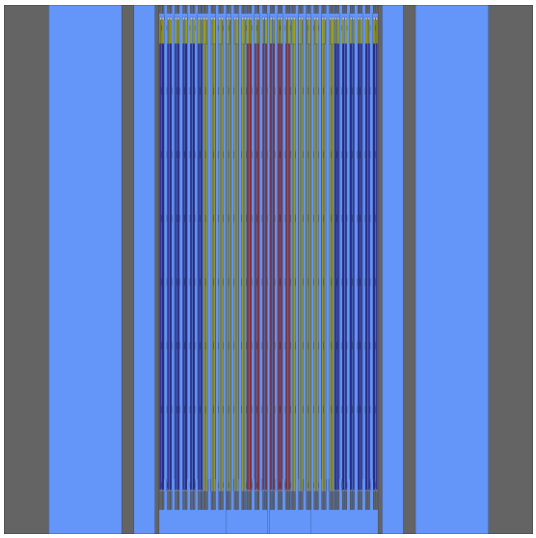
3. Results and Discussion

The correction ratios introduced within this study, devised to account for burnup effects, are subjected to validation within a 5*5 tiny reactor model. As shown in Fig. 9, this diminutive core configuration encompasses 21 fuel assemblies, enveloped by a reflective layer enshrouding them. The 21 assemblies encompass 5 red assemblies characterized by an enrichment of 1.6%, 4 yellow assemblies enriched to 2.4%, and 12 blue assemblies with an enrichment of 3.1%. The absence of control rod insertion is noted, and vacuum boundary conditions are assumed. The core undergoes burnup extending to 600 days at a power density of 23 kW/kg. Notably, benchmarking against computations utilizing the validated Serpent code is employed as the reference solution.

The outcomes of the computations are graphically depicted in Fig. 10. The reference solution is computed using the validated Monte Carlo code, Serpent, with an uncertainty of 1.1%. Following the application of the correction ratio, there is a notable reduction in the magnitude of both the k_{eff} error and the root-mean-square error (RMSE) associated with fission rate distribution.



(a) x-y plane view



(a) x-z plane view

Fig. 9. 5*5 tiny reactor model.

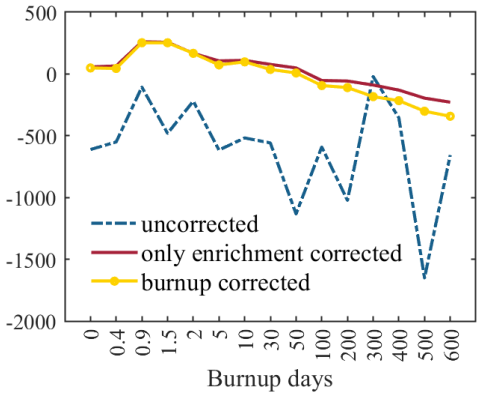


Fig. 10. k_{eff} error of different correction cases(pcm).

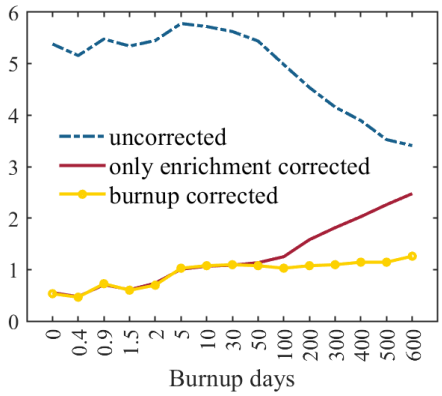


Fig. 11. Root-mean-square error of fission rate distribution in different correction cases (%).

It is observed that the uncorrected k_{eff} error comes quite insignificant when burn up to 300 days. This phenomenon arises due to the mutual counterbalancing of positive and negative errors in the fission rate, coincidentally reflecting in k_{eff} and creating the illusion of diminished error magnitude. However, a deeper analysis, as evident in Fig. 11, reveals that the RMSE persists at approximately 4.1%. This finding indicates that an obvious discrepancy still exists between the fission source distribution and the reference solution.

Furthermore, it is essential to recognize that the seemingly favorable outcomes obtained solely through the implementation of enrichment correction ratios is not enough. The cause for this illusion is the same as mentioned above.

It is evident that even with the application of correction ratios, the k_{eff} error still exceeds 340 pcm as the burnup progresses to deeper levels. This outcome does not reflect a desirable level of accuracy. Regarding this observation, two conjectures can be put forth. Firstly, during the actual burnup of the core, due to the non-uniform distribution of fission rates, each assembly experiences varying burnup powers that do not equate to the average power density as depicted in the database. Yet, during calculations, this work solely employs databases from single-power scenarios, neglecting the interpolation potential of multi-power databases. This discrepancy has the potential to introduce errors. Secondly, a possible reason is that the reference solution divides burnup regions based on fuel pins, while the fission matrix combination is based on assembly divisions. The preparation of databases incorporating power considerations and the technique of fission matrices combined with fuel rod segmentation are ongoing endeavors.

From Fig. 11, obviously, the application of material correction ratios at low burnup levels does not exhibit a conspicuous differentiation from the direct utilization of enrichment correction ratios. This phenomenon arises from the prevailing influence of enrichment over burnup during low burnup phases, where the impact of burnup remains relatively subtle. However, as the burnup deepens, burnup progressively becomes the dominant factor. Sole reliance on enrichment correction ratios proves inadequate in mitigating the errors arising from the combination of fission matrices, leading to an outcome where the enrichment-corrected RMSE values increasingly approximate those without correction.

Under entirely uncorrected circumstances, the RMSE diminishes as the burnup advances. This trend can be attributed to the differential consumption rates of materials with varying enrichment levels. Materials with higher enrichments experience faster burnup, while those with lower enrichments exhibit slower consumption rates. As burnup proceeds, the disparity between the two narrows, contributing to a reduction in the errors introduced by fission matrix combination. This phenomenon serves to highlight the non-uniform distribution of power within the system.

Excluding the time required for database-related calculations, the computational speed of the 5*5 small-core model in this study is notably swift. The entirety of 15 burnup steps, encompassing zero burnup as well, is accomplished within a mere 5 minutes, with an average time of approximately 20 seconds per burnup step. This stands in significant contrast to Monte Carlo simulations that demand CPU time of up to 2800 minutes per step, reflecting a considerable enhancement in computational efficiency.

However, it should be pointed out that the current duration of the database preparation process is relatively prolonged. The construction of a fission matrix database for a single material and a single burnup step necessitates 1 criticality simulation and 39 fixed-source calculations, amounting to approximately 93 CPU hours. Similarly, the correction ratio database requires 5 fixed-source computations, approximately consuming 70 CPU hours. The computational methodology for database construction is still subject to refinement, such as the optimization of particle count and the exploration of swifter means to acquire source information than criticality calculations. It is pivotal to underscore that the database needs to be formulated only once and can cater to diverse core assembly models. This enduring value remains particularly pronounced for endeavors that necessitate multiple burnup calculations.

4. Conclusions

In order to enhance the efficiency of reactor burnup calculations, this study introduces a novel approach based on the combined fission matrix theory. The core concept of this approach revolves around the introduction of correction ratios encompassing both burnup and enrichment. This method expedites the generation of requisite fission matrix databases and correction ratio databases through a series of rapid fixed-source simulations. In practical applications, the databases can be queried and interpolated based on material properties, facilitating combination and

correction operations without recourse to Monte Carlo simulations.

The preliminary outcomes of the 5*5 tiny reactor burnup over 600 days indicate that the material correction ratios, incorporating both burnup and enrichment, substantially mitigate the errors introduced by the combination of fission matrices during the burnup process. The RMSE remains consistently below 1.3%, and the k_{eff} error remains consistently below 350 pcm. These findings establish the capability of the CFM method to achieve acceptable precision while facilitating rapid computations. In addressing the issue of elevated k_{eff} errors, two potential approaches are being explored — the consideration of fission matrix databases corresponding to distinct power levels and the alignment of matrix combination with fuel pin burnups. Ongoing efforts are directed towards the pursuit of these solutions.

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