A Stable Condition and Adaptive Diffusion Coefficients for the Coarse-Mesh Finite Difference Method

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Coarse-mesh finite difference (CMFD) method is a widely used numerical acceleration method. However, the stability of CMFD method is not good for the problems with optically thick regions. In this paper, a stability rule named the "sign preservation rule" in the field of numerical heat transfer is extended to the scheme of CMFD. It is required that the disturbance of neutron current is positively correlated with that of the negative value of flux gradient. A necessary condition for stability of the CMFD method is derived, an adaptive diffusion coefficient equation is proposed to improve the stability of CMFD method, and the corresponding revised CMFD method is called the rCMFD method. With a few modifications of the code, the rCMFD method was implemented in the hexagonal-Z nodal S_N (discrete-ordinates) solver in the NECP-SARAX code system. The rCMFD method and other similar acceleration methods were tested by three fast reactor problems which were obtained by modifying the hexagonal pitches of a benchmark problem. The numerical results indicated that the rCMFD method showed better stability than the traditional CMFD method and the artificially diffusive CMFD (adCMFD) method and a better convergence rate than the adCMFD method and the optimally diffusive CMFD (odCMFD) method for these fast reactor problems.

Keywords: stable condition, adaptive diffusion coefficients, rCMFD, acceleration method, stability, IFDF, nodal SN method

1 INTRODUCTION

The convergence rate (Kuzmin, 2010) of the source iteration (SI) (Adams and Larsen, 2002; Li et al., 2015b) is often low when solving the reactor neutron transport problem. Many acceleration methods (Adams and Larsen, 2002; Willert et al., 2014) have been developed to accelerate the iteration process, such as the extrapolation methods, the Krylov subspace methods, and the high-order/low-order (HOLO) methods which are usually found to be the most efficient (Kuzmin, 2010; Willert et al., 2014). Here, the HOLO methods refer to a series of acceleration methods with the same internal logic that employs proper coupling between high-order discretization and low-order discretization to obtain high-order accuracy and high convergence rate, such as the multigrid method (Wesseling, 1995), the partitioned-matrix (PM) method (Li et al., 2015b), the diffusion synthetic acceleration (DSA) method (Alcouffe, 1977), the coarse-mesh finite difference (CMFD) method (Smith, 2002), and so on (Adams and Larsen, 2002; Zhang, et al., 2018). Among them, the CMFD method and other similar methods which employ the neutron diffusion approximation for the low-order discretization

are widely used in solving the reactor neutron transport problem (Smith, 2002; Lee et al., 2014; Zhang et al., 2019; Xu et al., 2020; Hao et al., 2021; Chan and Xiao, 2021; Zhao et al., 2022; Zhou et al., 2022) in recent years. However, the traditional CMFD method tends to fail due to iterative divergence for reactors with optically thick regions.

By reducing the coarse mesh size of the diffusion problem, increasing the number of transport sweeps, and adding over relaxation factors (Li et al., 2015a; Jarrett et al., 2016), the stability (Kuzmin, 2010) of CMFD can be improved to a certain extent. Compared with the traditional CMFD method, the pCMFD method and its variants (Yuk and Cho, 2017; Zhang et al., 2019) have improved stability by using partial neutron currents to calculate the coupling factors between high-order discretization and low-order discretization. The artificially diffusive CMFD (adCMFD) (Jarrett et al., 2016) and the optimally diffusive CMFD (odCMFD) (Zhu et al., 2016) can also improve the stability of the traditional CMFD method by improving the diffusion coefficients. The lpCMFD (Wang and Xiao, 2018; Wang and Zhu, 2021) method improves the stability of CMFD by flux prolongation. Some analyses of the variants of CMFD are available (Zhu, et al., 2017; Wang and Zhu, 2021). The IFDF (Xu, et al., 2020; Xu, et al., 2022) method adopts a coupling scheme different from the CMFD method and adaptively adjusts the diffusion coefficients during the iterative process, which was found to have better stability than the CMFD and adCMFD.

A stability principle, sign preservation rule (Tao, 2001) also known as the positive coefficients rule (Patankar, 1980), is required to obtain a stable discrete scheme in the field of numerical heat transfer. Its connotation is that the positive disturbance introduced at any grid should have a positive impact on other grids, which is physically reasonable. Considering the CMFD method, we found that the traditional CMFD equation could not physically reflect the response relationship between neutron currents and neutron fluxes, which was believed to be at least one main reason that causes the divergence of the iterative acceleration process.

In this paper, the condition for diffusion coefficients at the mesh surface is derived to keep the positive correlation between the neutron current and the negative values of the flux gradient by observing the sign preservation rule, the adaptive diffusion coefficient equation for the CMFD method is proposed, and the traditional CMFD method is revised as the rCMFD method. The theoretical derivation is presented in **Section 2**, the numerical results of different acceleration methods for three fast reactor problems obtained by modifying the hexagonal pitches of a small fast reactor benchmark problem are presented in **Section 3**, and the discussion and conclusion of this work are presented in **Section 4**.

2 THEORETICAL DERIVATION

2.1 Source Iteration
For high-order discretization, the discrete orders of spatial and angular dimensions of the neutron transport equation are high enough to give high accuracy. Taking the S_N method based on
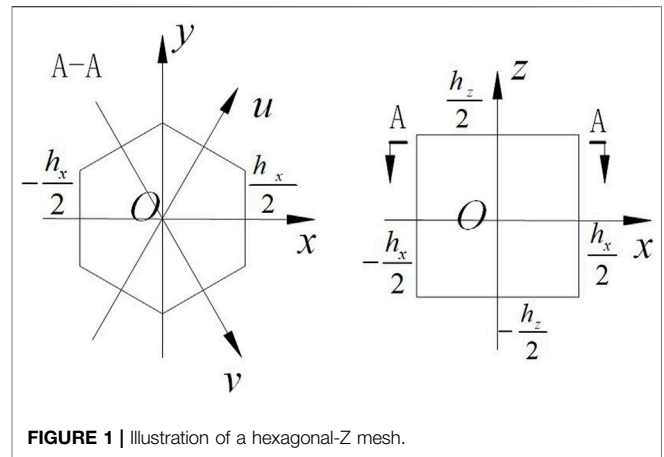

FIGURE 1 | Illustration of a hexagonal-Z mesh.

hexagonal-Z meshes as an example, the k-eigenvalue problem can be written as

$$L\psi = S\phi + \frac{1}{k}F\phi, \qquad (1)$$

where L is the neutron leakage matrix, ψ is the angular flux vector of every energy group, every spatial moment, and every discrete angle, S is the neutron scattering matrix, ϕ is the scalar flux vector, k is the eigenvalue, and F is the neutron fission matrix. The scalar flux vector could be calculated by the angular flux vector with

$$\phi = T\psi, \qquad (2)$$

where T is a matrix to calculate the scalar flux vector ϕ with the angular flux vector ψ. **Eqs 1**, **2** constitute the k-eigenvalue equations with high-order discretization, which could be solved by the classical power iteration also known as fission SI for the reactor problem:

$$\psi^{(n)} = \frac{1}{k^{(n-1)}}(L - ST)^{-1}F\phi^{(n-1)}, \qquad (3)$$

$$\phi^{(n)} = T\psi^{(n)}, \qquad (4)$$

$$k^{(n)} = k^{(n-1)}\frac{\langle F\phi^{(n)}\rangle}{\langle F\phi^{(n-1)}\rangle}, \qquad (5)$$

where the superscript (n) or (n-1) is the iteration index and the symbol $\langle\ \rangle$ means integration over the phase space with the energy, angular, and spatial dimensions. The dimension of the matrix $(L - ST)$ is usually very large, and its inverse is usually not conducted by direct matrix operation but achieved by transport sweeps of every mesh, angle, and energy group for the S_N method.

2.2 Traditional Coarse-Mesh Finite Difference Method
The stability of source iteration is good, but the convergence rate is usually low especially for large reactor problems. The CMFD acceleration method is commonly used in the solution of the S_N k-eigenvalue problem. In the process of source iteration, the k-eigenvalue problem of transport corrected finite difference diffusion equation (low-order discretization) is solved to correct the high-order iterative variables.

For a hexagonal-Z mesh as illustrated in **Figure 1**, the low-order neutron balance equation for every group to be solved can be written as

$$\sum_{d=v,x,u,z} \left(J_{K_d+1/2} - J_{K_d-1/2} \right) A_{K_d} + \Sigma_{r,K} \phi_K V_K = Q_K V_K, \quad (6)$$

where d is the dimension index with the possible values of v, x, u, z as illustrated in **Figure 1**, $J_{K_d\pm1/2}$ is the normal neutron current at the mesh surface indexed by $K_d \pm 1/2$, A_{K_d} is the surface area of mesh K along dimension d, $\Sigma_{r,K}$ is the removal cross section of mesh K, ϕ_K is the scalar neutron flux of mesh K, V_K is the volume of mesh K, and Q_K is the neutron source of mesh K including the fission source and scattering source from other groups.

For the CMFD method, the neutron currents and neutron fluxes in **Eq. 6** are related by the transport corrected Fick's law. For an inner mesh surface,

$$J_{K_d+1/2} = -\frac{D_{K_d+1/2}}{h_{K_d+1/2}} \left(\phi_{K_d+1} - \phi_K \right) - \frac{r_{K_d+1/2}}{h_{K_d+1/2}} \left(\phi_{K_d+1} + \phi_K \right), \quad (7)$$

where

$$D_{K_d+1/2} = \frac{2 D_K D_{K_d+1} h_{K_d+1/2}}{h_{K_d} D_{K_d+1} + h_{K_d+1} D_K}, \quad (8)$$

$$r_{K_d+1/2} = -\frac{h_{K_d+1/2} J_{K_d+1/2}^{SN} + D_{K_d+1/2} \left(\phi_{K_d+1}^{SN} - \phi_K^{SN} \right)}{\phi_{K_d+1}^{SN} + \phi_K^{SN}}, \quad (9)$$

$$h_{K_d+1/2} = \frac{1}{2} \left(h_{K_d} + h_{K_d+1} \right), \quad (10)$$

where $D_{K_d+1/2}$ is the common diffusion coefficient at the mesh surface, $r_{K_d+1/2}$ is the transport correction factor, h is the mesh size, and the superscript SN means the value is from the high-order transport calculation. For the boundary cases, take the mesh surface in the positive coordinate direction of mesh K as an example:

$$J_{K_d+1/2} = \frac{D_{K_d+1/2}}{h_{K_d+1/2}} \phi_K - \frac{r_{K_d+1/2}}{h_{K_d+1/2}} \phi_K, \quad (11)$$

where

$$D_{K_d+1/2} = \frac{2 D_K \alpha_{K_d+1/2} h_{K_d}}{\alpha_{K_d+1/2} h_{K_d} + 2 D_K}, \quad (12)$$

$$r_{K_d+1/2} = -\frac{h_{K_d+1/2} J_{K_d+1/2}^{SN} - D_{K_d+1/2} \phi_K^{SN}}{\phi_K^{SN}}, \quad (13)$$

in which $\alpha_{K_d+1/2}$ is the boundary parameter and equals 0 for the reflective boundary condition and 0.5 for the vacuum boundary condition.

Eqs 6–13 and the boundary equations for other cases constitute the coarse-mesh finite difference equations and can be solved with a linear solver for every group. Then, the low-order k-eigenvalue problem could be solved by source iteration or other more efficient algorithms. Details of the solution algorithm for the linear system with low-order discretization are not to be introduced here for simplicity. Finally, the iterative variables including k and scalar fluxes from high-order discretization are to be corrected:

$$k = k^{DIF}, \quad (14)$$

$$\phi_{i,K} = \phi_{i,K}^{SN} \frac{\phi_K^{DIF}}{\phi_{0,K}^{SN}}, i \geq 0, \quad (15)$$

where the superscript DIF means the value is the solution of the diffusion problem and the subscript i is the expansion order of the spatial moment for the nodal S_N method.

2.3 A Stable Condition and Adaptive Diffusion Coefficients

The convergence rate of the CMFD method is usually high. However, the stability of the CMFD method is a problem for the transport problem with optically thick regions. Let us check the CMFD equations from the stability rule in the field of numerical heat transfer. For an inner mesh surface, the traditional Fick's law without transport correction can be written as follows:

$$J_{K_d+1/2} h_{K_d+1/2} = -\phi_{K_d+1} D_{K_d+1/2} + \phi_K D_{K_d+1/2}. \quad (16)$$

It is seen that the mesh-surface diffusion coefficient $D_{K_d+1/2}$ is always positive from **Eq. 8**, which means that $J_{K_d+1/2}$ will always decrease when ϕ_{K_d+1} increases and always increase when ϕ_K increases. This phenomenon obeys the physical law of diffusion and should be established in the transport corrected cases. Let us check the case of CMFD by rewriting **Eq. 7** for inner mesh surfaces as follows:

$$J_{K_d+1/2} h_{K_d+1/2} = -\phi_{K_d+1} \left(D_{K_d+1/2} + r_{K_d+1/2} \right) + \phi_K \left(D_{K_d+1/2} - r_{K_d+1/2} \right). \quad (17)$$

From **Eqs 8, 9** it is seen that the coefficient $\left(D_{K_d+1/2} + r_{K_d+1/2} \right)$ of ϕ_{K_d+1} and the coefficient $\left(D_{K_d+1/2} - r_{K_d+1/2} \right)$ of ϕ_K are not guaranteed to be always positive, which means that the physical law of diffusion could not be guaranteed. So, the following conditions are required:

$$D_{K_d+1/2} + r_{K_d+1/2} > 0, \quad (18)$$

and

$$D_{K_d+1/2} - r_{K_d+1/2} > 0. \quad (19)$$

After substituting **Eq. 9** into **Eqs 18, 19**, the condition becomes

$$D_{K_d+1/2} > \frac{h_{K_d+1/2}}{2} \max \left(-\frac{J_{K_d+1/2}^{SN}}{\phi_{K_d+1}^{SN}}, \frac{J_{K_d+1/2}^{SN}}{\phi_K^{SN}} \right). \quad (20)$$

Then, let us check **Eq. 11** for the boundary cases; the following condition is obtained with similar derivation to the case of inner mesh surfaces:

$$J_{K_d+1/2}^{SN} > 0. \quad (21)$$

This condition is always met for the vacuum boundary condition. For the reflective boundary condition, nothing is required to meet the diffusion law since $J_{K_d+1/2} \equiv 0$. If the boundary surface is in the negative coordinate direction of mesh K, the response condition between the mesh-surface current and the mesh flux is also always met. All in all, only the condition of **Eq. 20** of the inner mesh surface is necessary.

FIGURE 2 | Flowchart of the rCMFD acceleration method.
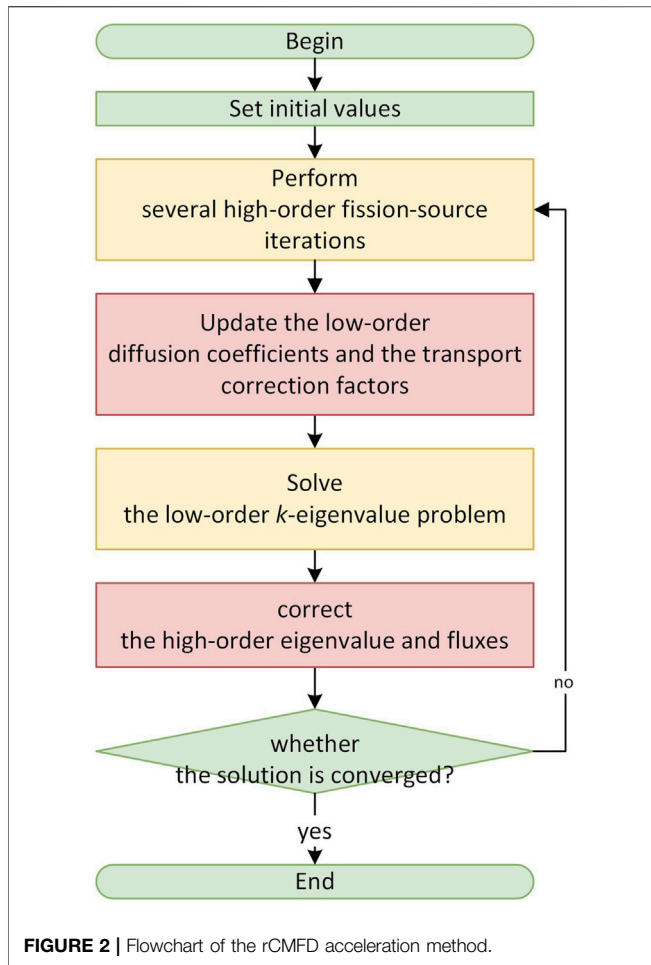
An interesting thing was found that **Eq. 20** was very similar to the stability equation of the IFDF method (Xu et al., 2020; Xu et al., 2022) which had been found to be more stable than the traditional CMFD method and the adCMFD method for a large fast reactor core. For one-dimensional (1D) meshes, the stability condition of the IFDF method is

$$D_K > \frac{h_K}{2} \max\left(-\frac{J_{K_d-1/2}^{SN}}{\phi_K^{SN}}, \frac{J_{K_d+1/2}^{SN}}{\phi_K^{SN}} \right). \quad (22)$$

The difference is in the subscripts, and the condition for the diffusion coefficient at the mesh surface becomes the condition for the diffusion coefficient in the mesh.

In order to guarantee the condition in **Eq. 20**, **Eq. (8)** is modified to the following equation of adaptive diffusion coefficient:

$$D_{K_d+1/2} = \max\left[\frac{2D_K D_{K_d+1} h_{K_d+1/2}}{h_{K_d} D_{K_d+1} + h_{K_d+1} D_K}, \frac{ch_{K_d+1/2}}{2} \right.$$
$$\left. \max\left(-\frac{J_{K_d+1/2}^{SN}}{\phi_{K_d+1}^{SN}}, \frac{J_{K_d+1/2}^{SN}}{\phi_K^{SN}} \right) \right], \quad (23)$$

where c is an additional damping parameter which should be larger than 1. With c larger than 1, **Eq. 23** gives a conservative condition to satisfy **Eq. 20**, and a larger value of c tends to increase the stability but decrease the convergence rate from our numerical tests. A value of 5 is recommended for c referring to the IFDF method and will be employed in the numerical tests of next section. When **Eq. 20** is met, the traditional mesh-surface diffusion coefficient in **Eq. 8** is employed to guarantee diagonal dominance of the low-order linear system, which will improve the solution speed of the low-order linear system; when **Eq. 20** is not met, **Eq. 23** will adaptively abandon **Eq. 8** and employ a more conservative mesh-surface diffusion coefficient equation in **Eq. 23** to meet the stable condition of **Eq. 20**.

Employing **Eq. 23**, the traditional CMFD method is improved to the revised CMFD (rCMFD) method. Few changes are needed to modify a CMFD acceleration process to an rCMFD acceleration process. What we should do is to replace **Eq. 8** with **Eq. 23** and update the mesh-surface diffusion coefficients before solving the low-order k-eigenvalue problem. The process of the rCMFD method is illustrated in **Figure 2**.

3 NUMERICAL RESULTS

3.1 Description of the Tests

Three fast reactor core problems were employed to test the methods. The first one (core 1) is a small fast reactor benchmark problem with hexagonal assemblies (Takeda and Ikeda, 1991). The hexagonal pitches are 12.9904 cm, and the total height of the model is 190 cm. Four-group cross sections are provided by the benchmark for different regions of the core. The case of half-inserted control rods is employed. The radial layout of the core is presented in **Figure 3**. The second one (core 2) and the third one (core 3) are obtained by changing the hexagonal pitches of core 1 to 50 and 100 cm, respectively, which may be not very rational for reactor design but helpful to test the convergence of numerical methods for problems with optically thick meshes.

The three problems have been calculated by the DNTH (Wang et al., 2020) solver in the NECP-SARAX (Zheng et al., 2018) code system with different methods including pure fission-source iteration (SI), fission-source iteration with CMFD acceleration (SI-CMFD), fission-source iteration with adCMFD ($\eta = 1/4$) acceleration (SI-adCMFD), fission-source iteration with odCMFD acceleration (SI-odCMFD), fission-source iteration with IFDF acceleration (SI-IFDF), and fission-source iteration with rCMFD acceleration (SI-rCMFD). The NECP-SARAX code system is a code system developed at Xi'an Jiaotong University for the neutronics analysis of advanced fast-spectrum reactors or facilities. The DNTH solver is an S_N nodal transport solver in NECP-SARAX for hexagonal-Z meshes with the capacity of large-scale parallel computing.

For all the cases, S_4 Legendre–Chebyshev angular quadrature was used; the number of hexagonal-Z meshes was 169×33; the nodal interior variables were expanded with second-order polynomials; the nodal surface variables were expanded with first-order polynomials; the fission-source iteration criterion of high-order discretization was 1×10^{-5}; the scattering-source iteration criterion of high-order
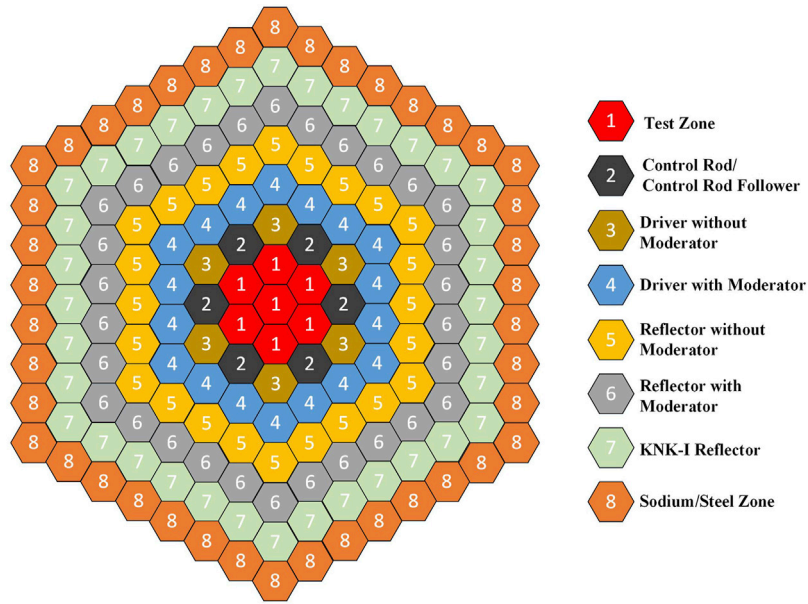
FIGURE 3 | Radial layout of the small fast reactor core.

TABLE 1 | Numerical results of the tests for different methods.

Item		SI	SI-CMFD	SI-adCMFD	SI-odCMFD	SI-IFDF	SI-rCMFD
Core (12.9904 cm pitches)	k_{eff}	0.98362	0.98368	0.98361	0.98363	0.98368	0.98368
	CPU time (s)	49	18	25	20	18	18
	Fission iteration count	81	29	43	37	29	29
	Transport sweep count	1480	518	687	586	523	518
	Speedup	1.0	2.7	2.0	2.5	2.7	2.7
Core 2 (50 cm pitches)	k_{eff}	1.48319	Divergent	Divergent	1.48310	1.48308	1.48311
	CPU time (s)	157			69	58	64
	Fission iteration count	253			101	90	98
	Transport sweep count	4922			1971	1736	1895
	Speedup	1.0			2.3	2.7	2.5
Core 3 (100 cm pitches)	k_{eff}	1.64874	Divergent	Divergent	Divergent	1.64843	Divergent
	CPU time (s)	240				121	
	Fission iteration count	383				177	
	Transport sweep count	7500				3453	
	Speedup	1.0				2.0	

discretization was 5×10^{-6}; an iteration limit of 5 was employed for the inner scattering-source iteration; the fission-source iteration criterion of low-order discretization was 2.5×10^{-6}; one low-order linear system was solved before four high-order fission-source iterations were performed. All the calculations were performed on 2.0 GHz AMD Ryzen PRO 2500U w CPU core.

3.2 Results for Different Cases
The results for the three reactor cores are presented in **Table 1**. In the table, one transport sweep means one update of all the mesh angular fluxes within one group, which is the main part of the time-consuming calculations, and the speedups are obtained by comparing the CPU time of every method with that of the SI scheme.

As shown in **Table 1**, for core 1, the radial hexagonal pitches were 12.9904 cm, and every method could give a convergent result; there were some deviations between the k_{eff} of different methods, which was caused by the different convergence degrees of the inner scattering-source iteration; the speedup of SI-rCMFD was 2.7, which was higher than those of adCMFD and odCMFD and close to those of SI-CMFD and SI-IFDF. For core 2, the radial hexagonal pitches were 50 cm, SI-CMFD and SI-adCMFD failed to converge, while SI, SI-odCMFD, SI-IFDF, and SI-rCMFD proposed in this work still could give convergent results; the speedup of SI-rCMFD for core 2 was 2.5, which was a bit lower than 2.7 of SI-IFDF but higher than 2.3 of odCMFD. For core 3, the radial hexagonal pitches were 100 cm, SI-rCMFD also failed to converge, and only SI and SI-IFDF could give convergent results.

4 DISCUSSION AND CONCLUSION

After numerical tests of three fast reactor problems with different radial hexagonal pitches from 12.9904 to 100 cm by different acceleration methods, the advantages and limitations of the proposed rCMFD method were clarified. It was seen that the adaptive diffusion coefficients of this work were helpful to improve the stability of the traditional CMFD method without obvious loss of the convergence rate, and the improvement was even higher than those of the adCMFD method and the odCMFD method which had been found to be more stable than the traditional CMFD method. However, the rCMFD method failed for the third core with radial hexagonal pitches of 100 cm, while the IFDF method still could give a convergent result with a speedup of 2.0, which indicated that the rCMFD was still not unconditionally stable and the stable region was narrower than that of the IFDF method although the adaptive diffusion coefficient equations were similar for the rCMFD and IFDF. The inferiority of the rCMFD method compared with the IFDF method may be due to the fact that Fick's law correction formula of the IFDF method is derived from the interface discontinuity relationship with clear physical significance, but Fick's law correction formula of rCMFD is based on a heuristic hypothesis as the traditional CMFD method.

It is concluded that the stable condition derived in this work is necessary for the CMFD stability but perhaps not sufficient for unconditional stability, and the adaptive diffusion coefficients can effectively improve the stability of the traditional CMFD method without obvious loss of the convergence rate. Further research on spectral radius analysis of the rCMFD method and comparison between different methods is expected, which may enlighten sufficient stable conditions or higher improvements of the CMFD method.

DATA AVAILABILITY STATEMENT

The original contributions presented in the study are included in the article/supplementary material, and further inquiries can be directed to the corresponding author.

AUTHOR CONTRIBUTIONS

ZX performed the methods and presented the results. HW supervised the work. YZ and QZ were advisers.

ACKNOWLEDGMENTS

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