Efficient Procedure For Radial MOC and Axial SN coupled 3D Neutron Transport Calculation

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Abstract - *The radial MOC and axial SN coupled method can achieve high precision 3D neutron transport calculation through direct angular flux coupling. However, it usually converges slowly and limits its engineering application. This article presents a new efficient procedure for 2D MOC and 1D SN coupled 3D neutron transport to converge rapidly and overcome the instability within it. It is realized by leakage terms converging in outer iteration, adjusted 3D CMFD acceleration and twice SN sweeps for each MOC sweep. This article briefly introduced 2D/1D coupling and acceleration theory, the efficient procedure for 2D MOC and 1D SN coupling, and the ways to make the calculation stable. The accuracy and efficiency of this procedre is verificated with 3D C5G7 extension case and prove to be practical.*

I. INTRODUCTION

KYCORE is a radial MOC and axial SN coupled 3D neutron transport software. It is based on a 2D MOC code KYLIN-2[1][2], which is developed by China Institute of Nuclear Power. Of all 2D/1D coupling[3][4][5][6][7], We choose 2D MOC and 1D SN coupled method[8][9][10]as it can realize high precision 3D neutron transport calculation through direct angular flux coupling. However, KYCORE is for future engineering application but MOC/SN coupled method usually takes too much calculation time for MOC/SN coupling to converge. So we make a procedure for radial MOC and axial SN coupled 3D neutron transport to converge rapidly and stable. The main idea is that leakage source is treated the same way as fission and scattering source do, which means it will converge in outer iteration. This decrease the high order sweep times but makes CMFD acceleration begin without MOC/SN converges to a same stable status. To overcome it, ways are raised to make the calculation stable. The fission and scattering source in MOC and SN are made sure to be the same. The CMFD are limited to run properly and we use characteristic line format for all high order calculation. We also do verification work on the case we made and 3D C5G7 extension case[11][12]. The procedure we design for MOC/SN coupled method has no leakage source iteration in it. It is feasible and simplified the calculation procedure, making its time consuming acceptable and the calculation remian to be precise.

II. DESCRIPTION OF THE ACTUAL WORK

To present 2D/1D coupled model, we begin with the 3D neutron Boltzmann equation in cylindrical-coordinate system:

$$\xi_m \frac{\partial \psi_g(\mathbf{r},\mathbf{\Omega}_m)}{\partial r} + \eta_m \frac{\partial \psi_g(\mathbf{r},\mathbf{\Omega}_m)}{r\partial\theta} - \eta_m \frac{\partial \psi_g(\mathbf{r},\mathbf{\Omega}_m)}{r\partial\omega}$$
$$+ \mu_m \frac{\partial \psi_g(\mathbf{r},\mathbf{\Omega}_m)}{\partial z} + \Sigma_{t,g}(\mathbf{r})\psi_g(\mathbf{r},\mathbf{\Omega}_m) = Q_g(\mathbf{r},\mathbf{\Omega}_m) \quad (1)$$

where $\xi_m = e_r \cdot \mathbf{\Omega}_m$, $\eta_m = e_\theta \cdot \mathbf{\Omega}_m$, $\mu_m = e_z \cdot \mathbf{\Omega}_m$, $\mathbf{\Omega}_m$ is the neutron transport direction, e_r is the radial direction, e_θ is perpendicular to radial direction, e_z is the axial direction, Q_g is the total source, $\Sigma_{t,g}(\mathbf{r})$ is total cross section, ψ_g is angular flux.

We choose cylindrical-coordinate system as it is close to 2D/1D model and easy to analysis.

For 2D MOC equation, we assume the material remain in the $[z_{k-1/2}, z_{k+1/2}]$ and integral (1) in the axial direction, and divide mesh width Δz_k in both side, then we get:

$$\xi_m \frac{\partial \psi_{g,m,k}(\mathbf{r},\mathbf{\Omega}_m)}{\partial r} + \eta_m \frac{\partial \psi_{g,m,k}(\mathbf{r},\mathbf{\Omega}_m)}{r\partial\theta} - \eta_m \frac{\partial \psi_{g,m,k}(\mathbf{r},\mathbf{\Omega}_m)}{r\partial\omega}$$
$$+ \Sigma_{t,g}(\mathbf{r})\psi_{g,m,k}(\mathbf{r},\mathbf{\Omega}_m) = Q_{g,m,k}(\mathbf{r},\mathbf{\Omega}_m) - TL_{g,m,k}^{Axial}(r,\theta) \quad (2)$$

Where $TL_{g,m,k}^{Axial}(r,\theta)$ is the axial leakage source.The axial leakage term can be calculated in this way:

$$TL_{g,m,k}^{Axial}(r,\theta) = \frac{1}{\Delta z_k}\int_{z_{k-1/2}}^{z_{k+1/2}} \mu_m \frac{\partial \psi_g(\mathbf{r},\mathbf{\Omega}_m)}{\partial z}dz$$
$$= \frac{\mu_m}{\Delta z_k}\left[\psi_{g,m,k+1/2}(r,\theta) - \psi_{g,m,k-1/2}(r,\theta)\right] \quad (3)$$

Equation (3) will be solved in 1D SN.

Then in MOC, we only consider the angular flux changes in $\vec{r}$ direction, so (2) will come down to:

$$\xi_m \frac{\partial \psi_{g,m,k}(\mathbf{r},\mathbf{\Omega}_m)}{\partial r} + \Sigma_{t,g}(\mathbf{r}) \psi_{g,m,k}(\mathbf{r},\mathbf{\Omega}_m)$$

$$= Q_{g,m,k}(\mathbf{r},\mathbf{\Omega}_m) - TL^{Axial}_{g,m,k}(r,\theta) \tag{4}$$

Through integaling in axial direction, 3D neutron transport equation (1) change into radial 2D MOC equation. Equation (4) will be solved in 2D MOC with last axial leakage terms calculated in equation (3). $TL^{Axial}_{g,m,k}(r,\theta)$ is the leakage source in kth planar in m direction.

In the same way, we assume the material remain in the mesh p and integral (1) in the radial direction, divide the mesh area S in both side, the we get:

$$\mu_m \frac{d\psi^p_{g,m}(z)}{dz} + \Sigma_{t,g,p}(z)\psi^p_{g,m}(z) = Q^p_g(z) - TL^{Radial}_{g,m,p}(z) \tag{5}$$

Where $TL^{Radial}_{g,m,p}(z)$ is the radial leakage source. Similarly, equation (5) will be solved in 1D SN with last radial leakage terms. The final work will be giving a easy and common expression for radial leakage to calculate in arbitrary 2D geometry.

The radial leakage term can be presented in this way:

$$TL^{Radial}_{g,m,p}(z) = \frac{1}{S}\int \xi_m \frac{\partial \psi_{g,m,p,r}(\mathbf{r},\mathbf{\Omega}_m)}{\partial r} + \eta_m \frac{\partial \psi_{g,m,p,\theta}(\mathbf{r},\mathbf{\Omega}_m)}{r\partial \theta} - \eta_m \frac{\partial \psi_{g,m,p,\theta}(\mathbf{r},\mathbf{\Omega}_m)}{r\partial \omega} dS \tag{6}$$

Analogously, only consider the angular flux changes in $\vec{r}$ direction, thus $\psi_{g,m,p,\theta}(\mathbf{r},\mathbf{\Omega}_m)$ and ω will identically equal to zero, (6) will come down to:

$$TL^{Radial}_{g,m,p}(z) = \frac{1}{S}\int \xi_m \frac{\partial \psi_{g,m,p}(\mathbf{r},\mathbf{\Omega}_m)}{\partial r} dS \tag{7}$$

Then we define $\cos p_z = e_z \cdot \mathbf{\Omega}_m$, p_z is the included angle between neutron transport direction $\mathbf{\Omega}_m$ and axial direction e_z. Then we will have

$$\xi_m = \sqrt{1 - \cos p_z^2}\cos\omega = \sin p_z .$$

Finally, we consider $\int dS = \sum dl \int_{r_{in}}^{r_{out}} dr$ may be suitable for all the arbitrary geometry of mesh p, where dl is the ray spacing.

Now the radial leakage term can be calculated in this way:

$$TL^{Radial}_{g,m,p}(z) = \Sigma \frac{\sin p_z dl}{S}\int \frac{\partial \psi_{g,m,p}(\mathbf{r},\mathbf{\Omega}_m)}{\partial r} dr$$

$$= \Sigma \frac{\sin p_z dl}{S}[\psi_{g,m,p+\frac{1}{2}}(z) - \psi_{g,m,p-\frac{1}{2}}(z)] \tag{8}$$

Through integaling in radial direction, 3D neutron transport equation (1) change into axial 1D SN equation. Equation (5) will be solved in 1D SN with last radial leakage terms calculated in equation (8). $TL^{Radial}_{g,m,p}(z)$ is the leakage source in pth mesh in m direction.

Usually, the MOC ans SN coupled 3D neutron transport is accelerated with CMFD(odCMFD[13]).

The CMFD model is as following:

$$\sum_p (J_{g,p+\frac{1}{2},k}S^{p+\frac{1}{2},k} - J_{g,p-\frac{1}{2},k}S^{p-\frac{1}{2},k})$$

$$+ \sum_k (J_{g,p,k+\frac{1}{2}}S^{p,k+\frac{1}{2}} - J_{g,p,k-\frac{1}{2}}S^{p,k-\frac{1}{2}})$$

$$+ V^{p,k}\overline{\Sigma}_{rm,g,p,k}\overline{\phi}^{p,k}_g - V^{p,k}Q_{scat,g,p,i} = V^{p,k}Q_{fis,g,p,i} \tag{9}$$

Where $J_{g,p+\frac{1}{2},k}$ and $J_{g,p-\frac{1}{2},k}$ are the net current in radial direction, $J_{g,p,k+\frac{1}{2}}$ and $J_{g,p,k-\frac{1}{2}}$ are the net current in axial direction, $S^{p+\frac{1}{2},k}$ and $S^{p-\frac{1}{2},k}$ are the areas between coarse meshs in radial direction, $S^{p,k+\frac{1}{2}}$ and $S^{p,k-\frac{1}{2}}$ are the areas between coarse meshs in axial direction, $V^{p,k}$ is the mesh volumn, $\overline{\Sigma}_{rm,g,p,k}$ is the homogenized transport cross section.

We put scattering source on left side to accelerate CMFD calculation.

The parameters for calculation come from the equivalent homogenization:

$$\overline{\Sigma}_{x,p,k} = \frac{\sum_{j\in p,k}\Sigma_{x,j}\phi_j V_j}{\overline{\phi}_{p,k}V^{p,k}} \tag{10}$$

$$\overline{\phi}^{p,k}_g = \sum_{j\in p,k}\phi_j V_j \tag{11}$$

To keep the high order and low order coupled with each other, we shall ensure the net neutron current in transport and diffusion calculation is the same. The net current in high order is calculated as following:

$$J_{g,p\pm\frac{1}{2},k}S^{p\pm\frac{1}{2},k} = w_a w_{p_z}\sin a \sin p_z \delta_a h_k(\psi^p_{g,p\pm\frac{1}{2},k} - \psi^n_{g,p\pm\frac{1}{2},k})$$

$$J_{g,p,k\pm\frac{1}{2}}S^{p,k\pm\frac{1}{2}} = w_a w_{p_z}\cos p_z S_p(\psi^p_{g,p,k\pm\frac{1}{2}} - \psi^n_{g,p,k\pm\frac{1}{2}}) \tag{12}$$

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Where a and p_z present depression angle and polar angle, w is weight factor, δ_a is ray space, h_k is aixal height and S_p is radial area.

And the net current in low order is calculate in this way:

$$J_{g,p\pm\frac{1}{2},k}S^{p\pm\frac{1}{2},k} = \bar{D}_{p\pm\frac{1}{2},k}(\bar{\phi}_{p,k} - \bar{\phi}_{p\pm1,k}) + \hat{D}_p(\bar{\phi}_{p,k} + \bar{\phi}_{p\pm1,k})$$

$$J_{g,p,k\pm\frac{1}{2}}S^{p,k\pm\frac{1}{2}} = \bar{D}_{p,k\pm\frac{1}{2}}(\bar{\phi}_{p,k} - \bar{\phi}_{p,k\pm1}) + \hat{D}_k(\bar{\phi}_{p,k} + \bar{\phi}_{p,k\pm1}) \quad (13)$$

Where $\bar{D}_{p\pm\frac{1}{2},k}$ is the diffusion factor, $\hat{D}_p$ is the correction factor.

At last, we assume that the radio of the fine net flux in the coarse mesh is unchanged before and after the correction.

$$\phi_j^{(l+1)} = \phi_j^{(l+\frac{1}{2})} \frac{\bar{\phi}_g^{p,k(l+1)}}{\bar{\phi}_g^{p,k(l+\frac{1}{2})}} (j \in p,k) \quad (14)$$

$\phi_j^{(l+\frac{1}{2})}$ and $\phi_j^{(l+1)}$ is finite mesh flux before and after CMFD acceleration, $\bar{\phi}_g^{p,k(l+\frac{1}{2})}$ and $\bar{\phi}_g^{p,k(l+1)}$ is homogenized coarse mesh flux before and after CMFD acceleration.

In the past, we regard 2D MOC and 1D SN as a whole[14]. There are leakage and scattering source iteration between 2D MOC and 1D SN. The CMFD begin when 2D MOC and 1D SN converge to the same stable status. Then the flux calculated in CMFD will return to MOC and SN until it comes to converge. The procedure for radial MOC and axial SN coupled 3D neutron transport calculation is as following:
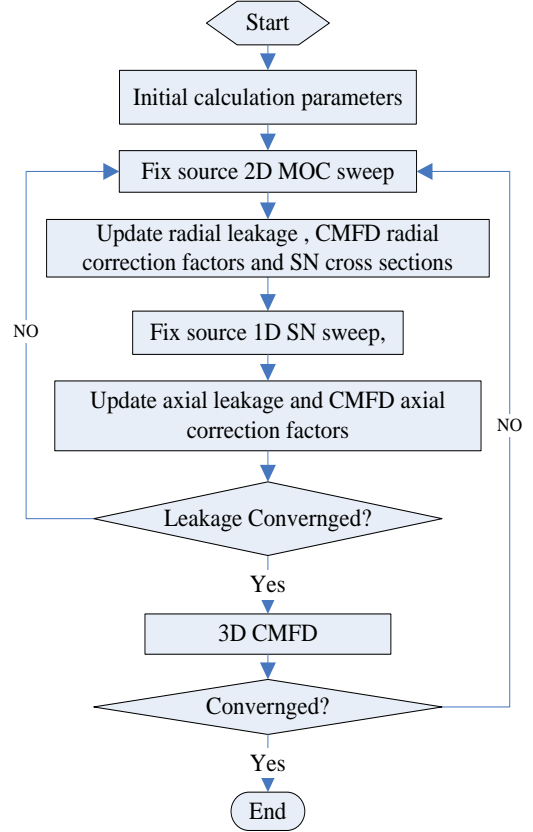

Fig.1. Former procedure for radial MOC and axial SN coupled 3D neutron transport calculation

The former procedure for radial MOC and axial SN coupled 3D neutron transport calculation is stable and precise. However, the source iteration between 2D MOC and 1D SN take too much time for convergency, which inspires us to improve it.

Oberseving (4)(5), the leakage source can regard as fission or scattering source, converging in outer iteration rather than in inner interation, which means MOC and SN can be solved relative independently and CMFD will accelerate both at the same time. Futhermore, (4)(5)indiciatied that MOC and SN share the same fission and scattering source. To ensure CMFD, MOC and SN calculate the same model, after CMFD iterations, MOC flux will be calculated with (13) and SN flux will be calculated as following：

$$\phi_{SN}^{p,k(l+1)} = \phi_{SN}^{p,k(l+\frac{1}{2})} \frac{\bar{\phi}_{CMFD}^{p,k(l+\frac{1}{2})}}{\bar{\phi}_{SN}^{p,k(l+\frac{1}{2})}} \frac{\bar{\phi}_{MOC}^{p,k(l+1)}}{\bar{\phi}_{CMFD}^{p,k(l+1)}} \quad (15)$$

$\phi_{SN}^{p,k(l+\frac{1}{2})}$ and $\phi_{SN}^{p,k(l+1)}$ is finite SN mesh flux before and after CMFD acceleration, $\bar{\phi}_{SN}^{p,k(l+\frac{1}{2})}$ is finite SN mesh flux homogenize on coarse mesh before CMFD

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acceleration, $\overline{\phi}_{CMFD}^{p,k(l+\frac{1}{2})}$ and $\overline{\phi}_{CMFD}^{p,k(l+1)}$ is coarse mesh flux before and after CMFD acceleration, $\overline{\phi}_{MOC}^{p,k(l+1)}$ is finite MOC mesh flux homogenize on coarse mesh after CMFD acceleration. We calculate SN flux in this way for making fission and scattering source in SN and MOC are the same in any case.

However, this makes leakage source converges slowly, so the acceleration for leakage source convergency in outer iterations is also in consideration.For each MOC sweep, there will be twice SN sweeps for more inner iteration times of each outer iteration.

Finally, the efficient procedure for radial MOC and axial SN coupled 3D neutron transport calculation we designed is as following:
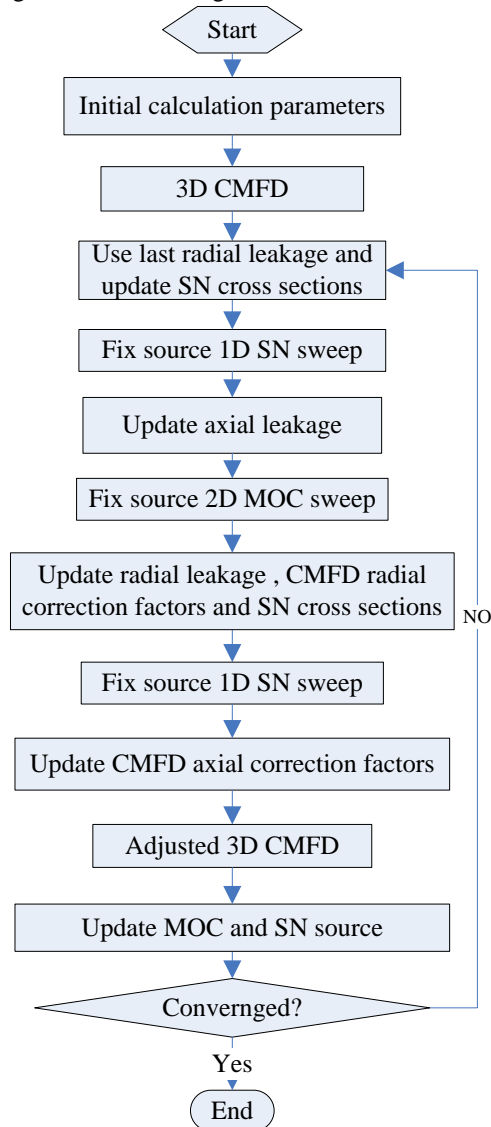

Fig.2. Efficient procedure for radial MOC and axial SN coupled 3D neutron transport calculation

In each circulation, we begin with the finite flux calculated in CMFD, then SN sweep for getting axial leakage source and axial correction factors, after that MOC sweep for getting radial leakage source and radial correction factors, then SN sweep again for more iteration times between MOC and SN, at last CMFD begin to accelerate the whole procedure. MOC consume the most time in a circulation, but in the circulation we designed MOC only sweep for once with fixed total source. In each MOC sweep, there are twice SN sweeps for leakage source acceleration and an adjusted 3D CMFD for fission and sacterring source acceleration. After CMFD, fission and sacterring source in MOC and SN will be updated at the same time for next circulation until converging.

As the leakage doesn't converge in high order during iteration and the 1D SN sweep calculation begin with old radial leakage source in the circulation. Sometimes 3D CMFD is unstable and hard to be solved. It may produce negative flux and diverge. Then we shall adjust 3D CMFD to run properly.

Above all, the diffusion factors $\overline{D}$ and correction factors $\widehat{D}$ will be limited to satisfy (13) and:

$$abs(\widehat{D}) \le \overline{D} \quad (16)$$

Apparently, it will prevent CMFD from getting negative flux.

Moreover, as the leakage terms don't converge in high order, the diffusion factors $\overline{D}$ and correction factors $\widehat{D}$ of CMFD are not always suitable. Sometimes we have to use damp factors for convergence, saying:

$$\widehat{D}^{(l+1)} = \delta\widehat{D}^{(l+\frac{1}{2})} + (1-\delta)\widehat{D}^{(l)} \quad (17)$$

However, $\delta = 1$ in default. It is not necessary in most cases.

Finally, the SN should better be calculated in characteristic line format instead of diamond format. The set 0 method in diamond format may cause CMFD acceleration disabled or oscillate. For example, in(12), if netcurrent $J = 0$ and surrounding flux $\overline{\phi}_s = 0$, then $\widehat{D} = -\overline{D}$, which is contradicted to the real model.

In radial mesh dividing, CMFD use the coarse meshs and each coarse mesh is divided into several MOC meshs for presicion calculation. In homogenized calculation, SN and CMFD share the same coarse mesh in radial direction. In heterogeneous calculation, SN and MOC share the same finite coarse mesh in radial direction.

In axial mesh dividing, a model is ofen divided into sevral MOC planar, each MOC planar use the same cross section, then each MOC planar is divided into several CMFD planars for acceleration and each CMFD planar is also divided into several SN planars for presicion calculation.

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III. RESULTS

The parallel work is not done with KYCORE, the calculation is in serial mode. The MOC/SN coupling permit heterogeneous fine calculation, but SN is calculated on homogenized coarse mesh as storage space limits.

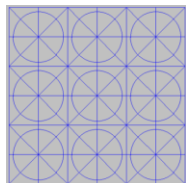To verify KYCORE efficency, we firstly test on a 3 * 3 PIN problem. The actual model is as following:

Fig.3. 3*3 PIN Problem

This benchmark is made by ourselves and KYCORE is verified with MCNP in this case. The PIN cell is made with water and UO2. It is 1.26cm in length and 20cm in height. All the boundary conditions are reflection except for the above ones, which are vacuum boundaries. The cross sections are in 7 groups.

The radial dividing is shown in Fig3. In axial dividing, we calculate 3*3 PIN problem with 2 planars for MOC calculation, each MOC planar has 10 CMFD planars for CMFD calculation and each CMFD planars has 10 SN planars for SN calculation.

The calculation result is as following:

Table 1 3*3 PIN Problem Calculation Result

	KYCORE	KYCORE(no acceleration)	MCNP
Keff	1.09736	1.09735	1.09712 ± 0.00027
MOC Sweep times	5	730	_
deviation/pcm	9	8	_

It can be seen that the acceleration in KYCORE have decrease the MOC sweep calculation for more than 100 times. Besides, the radial MOC and axial SN coupled 3D neutron transport has the comparable precision with MCNP.

However, only keff is in comparison in last case. Furthermore, we calculate the 3D C5G7 extension case for verification in keff and power. The 3D C5G7 extension case is 64.26cm in axial height and in radial length, which is the sum of 48.84cm for the fuel region and 21.42cm for the reflector region.

We calculate C5G7 Model with 4 MOC planars, each MOC planar is equally divided into 7,7,7 and 10 CMFD planars and each CMFD planar is equally divided into 10 SN planars. There are 6 polar angles for aixal direction and 20 depression angles for radial direcion. The calculation result is as following.

Table 2 3D C5G7 Case Keff Calculation Result

Benchmark mode	Un Rodded Case	Rodded A Case	Rodded B Case
Reference	1.14308	1.12806	1.07777
KYCORE	1.14313	1.12815	1.07732
MOC Sweep times	34	33	34
Time consuming(s)[a]	20302	19833	20547
deviation/pcm	5	9	45

a: The calculation is on Xeon E5-2650 within one core at 2 GHz

Table 3 3D C5G7 Case Power Calculation Result

Benchmark mode		Un Rodded Case	Rodded A Case	Rodded B Case
Slice 1	Maximum	1.367	1.726	1.360
Pin Power Error(%)	RMS	0.347	0.392	0.622
Slice 1	UO_2-1	0.373	0.379	0.419
Assembly Error(%)	MOC	0.156	0.315	0.641
	UO_2-2	0.121	0.048	0.573
Slice 2	Maximum	1.833	1.839	1.503

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Pin Power Error(%)	RMS	0.332	0.309	0.408
Slice 2 Assembly Error(%)	UO$_2$-1	0.163	0.140	0.518
	MOC	0.005	0.123	0.180
	UO$_2$-2	0.314	0.198	0.248
Slice 3 Pin Power Error(%)	Maximum	1.796	2.096	2.413
	RMS	0.727	1.132	1.513
Slice 3 Assembly Error(%)	UO$_2$-1	0.576	1.245	1.652
	MOC	0.381	0.953	1.296
	UO$_2$-2	1.012	1.349	1.801
Integrated Pin Power Error(%)	Maximum	1.349	1.514	1.284
	RMS	0.302	0.286	0.233
Integrated Assembly Error(%)	UO$_2$-1	0.109	0.082	0.069
	MOC	0.006	0.023	0.117
	UO$_2$-2	0.367	0.318	0.150

As is seen above, we calculate Un Rodded, Rodded A and Rodded B cases. The keff and pin power are in comparison.

It can be seen that the calculation on c5g7 extension case is about 5.5h and each outer iteration is about 10 min. The efficient procedure adds outer iteration times but decrease the outer iteration time-consuming dramatically. Comparing to former procedure, the effient of MOC/SN coupling obvious decrease the total calculation time. On the other hand, it can be seen from the power and keff comparison that the precision of MOC/SN coupling remain relative satisfactory. The leakage source convergency between MOC and SN is not nessecary for CMFD to acceleratioin. It can be infered that although the efficient procedure only mainly accelerate fission and scattering sources, it also in turn accelerate leakage source as long as the fission and scattering sources in MOC and SN are ensured the same and CMFD can run properly. The main idea of the procedure we design is that the leakage soucrce convergency can be included in outer iteration. Although the convergency of MOC or SN isn't as good as former procedure do at the beginning, it can be infered from equation (4)(5) that leakage source mainly affect the areas where is pure scattering and close to vacuum boundary, the fuel area is relatively in right solution, and the correction factors calculated for CMFD is not affected by it very much. Moreover, when the iteration close to converge, MOC and SN in the efficient procedure also almost converge to the same stable status, giving a relative right solution for the CMFD converging as fast as it in former procedure do.

IV. CONCLUSIONS

Though leakage terms converging in outer iteration, adjusted 3D CMFD for fission and scattering source acceleration and twice SN sweeps for each MOC sweep to accelerate leakage source, we complete the MOC/SN coupled 3D neutron transport work with high efficient procedure for future engineering application.

The main idea of effient procedure is to have leakage soucrce convergency included in outer iteration. It is mainly designed to decrease the outer iteration time-consuming as MOC can only sweep once for each outer iteration without leakage terms converging well. It is realized by ensure the fission and scattering sources in MOC and SN are the same in any cases while they calculate in a relative independent way. And CMFD is limited to avoid having negative flux or becoming instable. The verification on c5g7 extension case give a relative satisfying result to prove the precision of KYCORE is reliable and the time consuming is acceptable. However, there some drawback with the procedure we design. The increase on outer iteration times inspire us to improve it. The relative error in some extrem case may be also decreased in the future by some means. Anyway, the basic transport work of KYCORE is available and lay a fundamention for its future development. The futher way to go in neutron transport part may focus on the approximation in 2D/1D method itself and overcome it.

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