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DECOUPLED PLANAR MOC SOLUITION FOR DYNAMIC GROUP CONSTANT GENERATION IN DIRECT THREE-DIMENSIONAL CORE CALCULATIONS

Yeon Sang Jung and Han Gyu Joo
Department of Nuclear Engineering, Seoul National University
San 56-1, Sillim-dong, Seoul, Korea
ny164@snu.ac.kr; joohan@snu.ac.kr

ABSTRACT

A decoupled planar method of characteristics (MOC) solution based direct three-dimensional (3-D) core calculation scheme is introduced as an effort to enhance the solution stability and accuracy of a hybrid transport solution scheme employing the MOC only to the radial solution. Each planar MOC problem is solved as an eigenvalue problem with the axial leakage converted into the pseudo absorption cross section. The MOC-generated cell homogenized group constants and the current correction factors which are to be used in the subsequent coarse mesh finite difference (CMFD) formulation are not iteratively updated unlike the coupled scheme. The resulting 3-D CMFD problem is thus solved as an isolated problem. The decoupled scheme is applied to the rodded problems of the C5G7MOX benchmark to show that the degradation of the solution accuracy is negligible while the gain in the computing time is significant.

Key Words: MOC, CMFD, Hybrid Transport, Pseudo Absorption, Decoupling

1. INTRODUCTION

In order to realize the capability of *direct* three-dimensional (3-D) core calculation which does not involve any advance generation of group constants, the planar method of characteristic (MOC) solution based whole core transport calculation method[1] was developed. This method was proven to be quite effective through the implementation into the DeCART code[2] which can perform direct whole core transport calculations with the subpin level thermal feedback. A synthetic combination of the radial 2-D MOC solution with a different type of axial 1-D transport solutions such as the diffusion or SPn based solution forms the base of this method. Similar 2-D/1-D synthetic combination methods have been examined and proved effective by other researchers as well[3,4].

In the current DeCART formulation, the radial MOC solution is coupled with the axial SP3[5] solution through the pin-cell based coarse mesh finite difference (CMFD) formulation[6]. In this formulation, the axial leakage information is iteratively updated using the solution of the 3-D CMFD problem in which the embedded SP3 solver produces the axial flux profiles. The pin-wise axial leakage information is then fed into each planar MOC problem as an independent source. The pin-cell homogenized group constants and radial current correction factors resulting from the planar MOC calculations are used in the subsequent 3-D CMFD calculation. Therefore, the planar MOC problems are coupled tightly with the 3-D CMFD problem and thus simultaneous

solutions need to be obtained for both MOC and CMFD problems through the repeated alternate calculations of the two problems.

In the direct whole core calculation to be performed for power generating conditions, the subpin level temperature and coolant density distributions have to be determined concurrently with the flux distribution. Since the thermal condition is not fixed and it is gradually converging, the planar MOC calculation as well as the 3-D CMFD calculation has to be performed repeatedly with the changing cross sections incorporating thermal feedback. This poses a significant computational burden particularly on the planar MOC calculation which takes the most computing time and thus hinders practical applications of the direct whole core calculation to routine design analysis. The motivation for this work is to alleviate the computational burden for the planar MOC calculation by devising a decoupled calculation scheme through which a functionalization of dynamically generated pin-cell group constants is possible so that only 3-D CMFD calculation can be performed afterwards to determine the power distributions with thermal feedback.

2. DECOUPLED PLANAR MOC BASED 3-D CMFD CACLULATION

The coupled planar MOC based 3-D CMFD calculation scheme is a well-established formulation for efficient direct 3-D whole core calculation requiring mutual exchange of information between the two solution modules for a consistent solution of the neutron balance at each pin-cell level node. The CMFD nodal balance condition consisting of the leakages for all three directions as well as the source and removal terms should also be satisfied in the planar MOC calculations so that the axial leakage and the eigenvalue determined from the 3-D CMFD should be used in the MOC calculations. Conversely, the radial currents determined in the MOC calculations are to be satisfied in the 3-D CMFD calculation by forcing the current vs. cell average flux relation of the CMFD formulation to be the same as that obtained from the MOC calculation results. To guarantee the convergence of the alternate calculation of 3-D CMFD and planar MOC calculations, the consistency in the nodal balance condition must be maintained. This is a very strict requirement that may hinder the convergence performance of the coupled calculation. The decoupled scheme to be considered below is to relax this consistency condition by separating the planar MOC problems from the 3-D CMFD problem.

In the decoupled planar MOC based 3-D CMFD calculation scheme, the planar MOC only serves as an online group constant generator for the 3-D CMFD calculation. That means that each MOC plane solves a distinct 2-D plane-wise eigenvalue problem so that each planar problem has its own eigenvalue. The solution of 3-D eigenvalue problem is only obtained from the 3-D CMFD calculation. This can be possible by approximating the effect of axial leakage in the planar MOC by a pseudo absorption cross section. This is in contrast with the axial leakage used as the fixed source in the coupled scheme. In this scheme, the convergence of the global problem depends solely on that of the 3-D CMFD problem, meaning that the convergence is not affected by the intermediate planar MOC solutions.

While the radial mesh size is small in the 3-D CMFD problem due to the use of the pin-cell as the CMFD mesh, the axial mesh size is normally taken to be quite large, namely about 15~20 cm. The motivation for employing large axial meshes is to reduce the number of planes for

which the MOC calculations are to be performed and consequently to save the computing time. In order to describe properly the axial flux variation within a long mesh, a nodal method need to be used for the solution of the diffusion or the SP3 equation in the axial direction. In the following, the decoupled planar MOC and CMFD formulation is detailed and an effective iteration scheme for the decoupled calculation is introduced.

2.1. Decoupled Planar MOC Formulation

Suppose a 3-D neutron transport problem of which the domain is divided into several radial planes. The transport equation for a discretized angle *m* can be integrated over the axial direction on a plane (designated by plane index *k*) to yield:

$$\left(\varepsilon_m \frac{\partial}{\partial x} + \eta_m \frac{\partial}{\partial y} \right) \bar{\varphi}_m^k(x,y) + \Sigma_{tr}^k(x,y) \bar{\varphi}_m^k(x,y) = \bar{Q}_m^k(x,y) - L_{z,k}^m(x,y) \tag{1}$$

where $\bar{\varphi}_m^k(x,y)$ and $\bar{Q}_m^k(x,y)$ are the axially averaged angular flux and source while $L_{z,k}^m(x,y)$ is the axial leakage defined as:

$$L_{z,k}^m(x,y) = \frac{\mu_m}{h_k} \left(\varphi_m^{T,k}(x,y) - \varphi_m^{B,k}(x,y) \right). \tag{2}$$

Here $\varphi_m^{T,k}$ and $\varphi_m^{B,k}$ are the angular fluxes at the top and bottom of the plane. Eq. (1) is the planar problem which can be solved by the 2-D MOC for each plane. In the planar MOC problem, the axial leakage term of Eq. (2) needs to be specified as an additional angle dependent source and it can be determined in an approximate manner from the diffusion or SP3 solution available from the 3-D CMFD results. In the coupled mode formulation, each planar MOC problem becomes a source problem.

The basic idea of decoupled scheme is to convert the MOC fixed source problem into an eigenvalue problem. To transform Eq. (1) into an eigenvalue problem, an approximation that can transform properly the independent source term into a term proportional to the eigenfunction is needed. By introducing a pseudo absorption cross section defined as:

$$\Sigma_k^l(x,y) = \frac{\sum_m w_m L_m^k(x,y)}{\sum_m w_m \bar{\varphi}_m^k(x,y)} \tag{3}$$

where w_m is the angular weights. Eq. (1) now can be converted into an eigenvalue problem where the transport cross section is increased by Σ_k^l. The introduction of the pseudo abosrption term yields a different eigenvalue for each planar problem.

The axial leakage term to be used in the determination of the pseudo absorption cross section is simply approximated following manner:

$$L_{z,k}^{m}(x,y) = \frac{J_m^{T,k} - J_m^{B,k}}{4\pi h_k} \tag{4}$$

where $J_m^{T,k}$ and $J_m^{B,k}$ are the net current at the top and bottom of the plane determined in the the 3-D CMFD calculation. These are the pin-cell-wise axial currents. Because of the use of the cell average value for the axial current, the flat source regions in the same pin cell share same pesudo absorption cross section. The same pseudo absorption cross section being used in all the regions within a cell is in full agreement with the use of the same axial leakage source in all the internal regions in the coupled mode which turned out to have insignificant impact in the final result of the eigenvalue and pin power distribution.

2.2. 3-D CMFD Formulations with Two-Node Axial SENM Kernel

The solution of each planar MOC problem can be used to generate cell-wise homogenized group constants including the radial current correction factor which specifies the CMFD relation for the cell interface current in terms of the two neighboring cell average fluxes. Since the pseudo absorption cross section for axial leakage is used in the planar MOC calculation, the resulting cell homogenized group constant can be regarded as a function of axial leakage. Once this functional dependence is etablished, the 3-D CMFD problem can be solved as an independent problem and the planar MOC problems serves as the homogenized cross section generator.

As mentioned earlier, the axial mesh sizes are relatively large compared with the radial meshes in the 3D CMFD formulation. The axial dependence of the flux within the node thus needs to be described by a higher order nodal method. When the diffusion equation is used axially, the nodal expansion method (NEM) was used in the DeCART code with the partial currents specified as the boundary condition at the top and bottom surfaces of a node. The axial partial current based implementation of NEM yields a plane-wise solution scheme in the 3-D CMFD calculation as well. The plane-wise solution scheme is also used in the case of SP3 kernel. The plane-wise solution scheme is not, however, an efficient solution scheme because it involves a Gauss-Seidel type updates of the axial partial current. This planar solution scheme of the 3-D CMFD makes sense in the coupled solution scheme because the planewise sweep is necessary for the MOC calculations anyway. In the decoupled scheme in which the 3-D CMFD should be solved independently, however, a better solution scheme is necessary that can converge faster with more robust convergence behavior. The two-node nodal solution approach can be the candidate for the axial nodal solution.

The Source Expansion Nodal Method (SENM) [7] is one of the semi-analytic nodal methods. It represents all the source terms as a quartic polynomial so that the analytic solution to the transverse-integrated 1-D diffusion equation can be obtained as the summation of the exponential functions and the polynomial functions for each group. The two-node SENM formulation is used here in which the node average fluxes of all groups determined from a 3-D CMFD solution are specified as the constraints to be conserved by the higher order nodal solution. The resulting SENM solution for the axial direction then gives the axial current correct factor which is to be

used in the subsequent 3-D calculation. Note that the radial current correction factors needed in the 3-D CMFD formulation are considered predetermined by the preceding planar MOC calculations. Thus the radial current correction factors remain constant during the CMFD calculation and only the axial ones are iteratively updated through the alternate calculations of the 3-D CMFD and two-node SENM calculations. The two-node SENM solution for the axial SP3 formulation to replace the diffusion solution is still underway.

2.3. Decoupled Calculation Flow

In the decoupled scheme, the planar MOC calculation needs to be done prior to the 3D CMFD calculation and the pseudo absorption cross section is needed to represent the axial leakage. The pseudo absorption cross section which should be a function of axial leakage can not be known, however, at the time of the first planar MOC calculation and it should be determined from the 3-D CMFD solution. An iterative scheme is thus necessary to determine the pseudo absorption cross section. It can be done in two steps. At first, the planar MOC calculation can be done without the pseudo absorption cross section to generate the first set of homogenized group constants. The subsequent 3-D CMFD calculation can then determine the axial leakage and the corresponding pseudo absorption cross section.

At the first planar MOC calculation, each planar problem needs to be solved as an eigenvalue problem. The need for solution of multiple eigenvalue problems requires two special considerations. The first one is to obtain the converged solution for each 2-D MOC problem including the converged planar eigenvalue. Because of the need for convergence of each planar problem, a separate acceleration scheme using 2-D CMFD is necessary. It turned out that about 5 ray tracing (RT) calculations are necessary for each planar MOC problem with the 2-D CMFD turned on. Noting that each planar MOC problem need not be solved completely at each MOC calculation step in the coupled mode and the convergence of the planar MOC solution is sought along with the 3-D CMFD solution, one might think that the need for the converged 2-D MOC solution might cause a waste of calculation. But this observation is true only when a single state calculation is to be done. If calculations for several states are to be done in one run as in the case of depletion or transient calculation, the computational load for the subsequent planar MOC calculation can be significantly reduced because a good initial guess of the MOC solution is already available from the previous 2-D MOC solutions. This possibility of the reduction in the number of RT calculations in the subsequent MOC calculations is verified by the number of RT of the second planar MOC calculation which are formulated with the pseudo absorption cross section after the first 3-D CMFD calculation. Only one or two RT calculations are necessary in the second MOC problem because the flat source region-wise scalar flux distribution obtained in the previous MOC calculation does not change much with the introduction of the pseudo absorption cross section representing the axial leakage. This fact will be verified later with practical examples. The second special consideration is needed for the reflector planes having no independent fission source so that an eigenvalue program cannot be constructed for the reflector plane only. In such case, a two-plane problem which includes the neighboring fuel plane as well.

The calculation scheme described above is schematically shown in Figure 1. Note that there are several layers shown for the planar MOC solution part signifying that this calculation should be

done for each plane. Once the group constants are all determined after two times of MOC solutions, the 3-D CMFD problem is solved in the isolated mode.

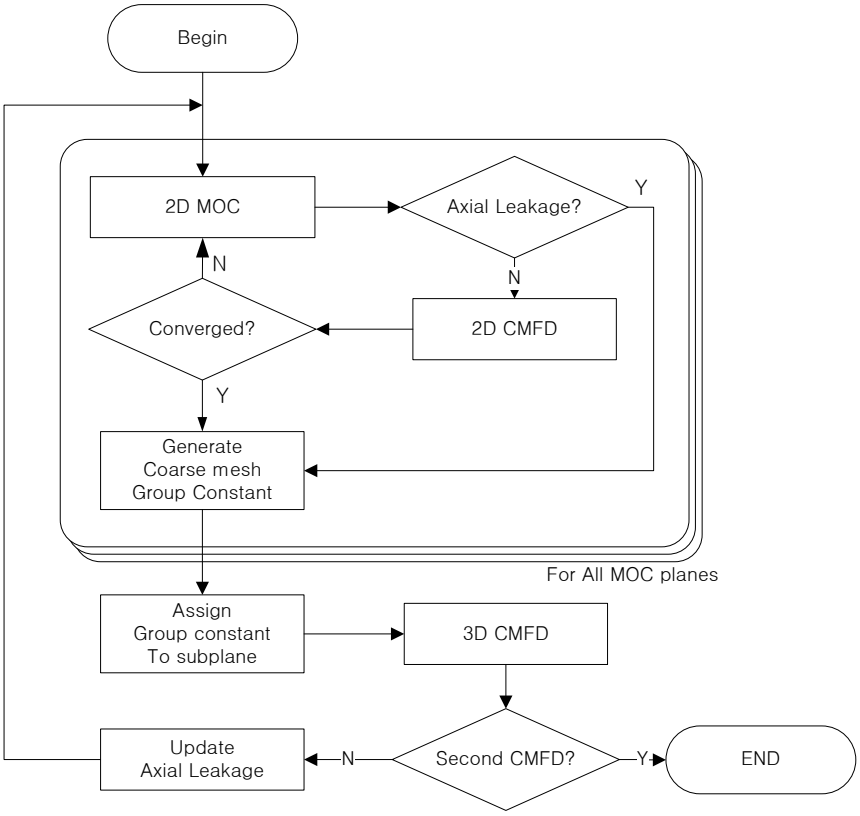

Figure 1. Decoupled Calculation Flow

In order to enhance the computational efficiency, the planar MOC can be performed with thick planes. This is feasible by noting that the axial leakage effect would have a less dominant effect in the cell homogenized cross sections generated than the radial heterogeneity effect. In this regard, the MOC calculations thus need to be performed only for the planes which have a different radial material configuration. The axial heterogeneity effect would then be treated in the 3D CMFD calculation with relatively thin axial meshes. This scheme is what is called the subplane method[6] or the coefficient sharing methods[4].

3. PERFORMANCE EXAMINATION

Both the coupled and decoupled planar MOC based 3-D CMFD calculation scheme have been implemented in a new 3-D whole core code named nTRACER. This code employes the assembly based modular ray tracing scheme for the planar MOC calculation and a two-node SENM for the axial diffusion calculation. The resonance calculation is performed using the subgroup method.

In order to examine the performance of the decoupled calculation, the C5G7MOX problems [8] were solved using the nTRACER code. Both the coupled and decoupled schemes were used to generate the base solutions for the three cases: Unrodded, Rodded A and Rodded B. In the base model, a large axial node size of 14.28 cm was used. This case is the 4 plane case. The nTRACER results obtained with the axial diffusion solver are given in Tables I though III. The first thing noted in these tables is that there is no considerable degradation in the solution accuracy with the use of the decoupled scheme even for the rodded cases. Particularly in the unrodded case, the accuracy of the decoupled solution is almost the same as that of the coupled case while a significant reduction in the RT computing time is saved by more than a factor of 3. The reduction in the RT computing time was possible by solving only one fuel plane out of the three planes in case of the decoupled scheme which takes the advantage of the uniform composition for the unrodded case. Thus only three sets of homogenized cross sections were sued in the decoupled calculation: the first for the interior fuel planes, the second for the peripheral fuel planes and the last for the reflector plane.

The effect of axial leakage on the homogenized pin cell cross section is expected to be much larger for the rodded cases. The results shown for the rodded cases, however, indicate that the difference in the accuracy between the coupled and decoupled cases is insignificant although slightly larger errors are noted for the decoupled cases. The largest slice pin power error noted for Rodded B at Slice 3 is 5.8% for the coupled case and the corresponding value for the decoupled case is 6.2%. This large error decreases with finer axial nodes. For the 16 plane case whose plane thickness is only the quarter of the base case, the error of the decoupled case (2.2%) is even smaller than the coupled case (2.8%). This seemingly unreasonable reversal of the error behavior would be due to some cancelation of errors. The insignificant difference in the solution error in this severely rodded problem implies that the effect of the axial leakage on the homogenized group constant is not that important signifying the decoupled solution approach is reasonable.

As shown in Tables II and III, the error decreases with the refinement of the axial mesh, at the expense of significantly increasing computing time for the coupled scheme. On the contrary, the computing time for the coupled scheme does not increase appreciably with the number of subdivision of the plane because the planar MOC calculations need to be performed only for the thick base planes and the same group constants can be used in multiple planes which share the same radial configuration.

Table I. Comparison of Coupled and Decoupled Solutions for Unrodded C5G7MOX

Calculation Mode		Coupled	Decoupled
Eigenvalue Error[1], pcm		36	38
Axially Integrated Pin Power Err. (%)	**Max.**	1.04	1.04
	Mean	0.30	0.31
	RMS	0.37	0.37
Computing Times (sec)	**RT**	1071.9	357.245
	CMFD	346.8	463.9

[1] Eigenvalue error ($\Delta\rho$) from the corresponding MCNP reference solution (1.18381)

Table II. Comparison of Coupled and Decoupled Solutions for C5G7MOX Rodded A

Calculation Mode		Coupled			Decoupled		
Axial Plane[1)]		4	8	16	4	8	16
Eigenvalue Error, pcm[2)]		-55	77	108	-59	73	105
Slice 1 Pin power Error (%)	Max.	1.77	1.17	1.43	1.82	1.12	1.34
	Mean	0.65	0.31	0.32	0.69	0.32	0.31
	RMS	0.75	0.38	0.41	0.79	0.39	0.40
Slice 2 Pin power Error (%)	Max.	1.32	1.43	1.55	1.28	1.42	1.48
	Mean	0.53	0.35	0.33	0.52	0.34	0.34
	RMS	0.62	0.43	0.42	0.61	0.42	0.43
Slice 3 Pin power Error (%)	Max.	2.99	1.81	1.84	3.39	1.97	1.75
	Mean	1.44	0.42	0.61	1.69	0.62	0.56
	RMS	1.67	0.55	0.72	1.95	0.73	0.66
Axially Integrated Pin Power Err. (%)	Max.	1.03	1.22	1.29	1.00	1.19	1.22
	Mean	0.27	0.29	0.31	0.26	0.26	0.31
	RMS	0.33	0.36	0.38	0.31	0.34	0.38
Computing Times (sec)	RT	530.8	832.8	1664.8	402.5	407.8	446.8
	CMFD	28.1	43.8	117.3	55.3	82.4	131.6

[1)] Number of sub division of the base axial mesh

[2)] Eigenvalue error ($\Delta\rho$) from the corresponding MCNP reference solution (1.12807)

Table III. Comparison of Coupled and Decoupled Solutions for C5G7MOX Rodded B

Calculation Mode		Coupled			Decoupled		
Axial Plane[1)]		4	8	16	4	8	16
Eigenvalue Error, pcm[2)]		-59	162	201	-72	149	187
Slice 1 Pin power Error (%)	Max.	1.74	2.04	2.00	1.78	1.80	2.25
	Mean	0.59	0.39	0.40	0.65	0.37	0.46
	RMS	0.73	0.52	0.52	0.79	0.49	0.59
Slice 2 Pin power Error (%)	Max.	1.31	1.93	2.21	1.47	2.14	2.07
	Mean	0.35	0.39	0.41	0.42	0.45	0.40
	RMS	0.44	0.53	0.58	0.54	0.59	0.55
Slice 3 Pin power Error (%)	Max.	5.84	2.83	2.77	6.23	3.34	2.21
	Mean	1.94	0.74	0.60	2.19	0.96	0.51
	RMS	2.52	0.95	0.77	2.76	1.20	0.66
Axially Integrated Pin Power Err. (%)	Max.	1.33	2.11	2.21	1.47	2.18	2.16
	Mean	0.31	0.39	0.38	0.32	0.40	0.39
	RMS	0.38	0.54	0.53	0.40	0.55	0.54
Computing Time (sec)	RT	610.5	943.6	1886.9	390.2	373.7	397.4
	CMFD	30.7	49.3	138.4	69.8	86.3	172.5

[1)] Number of sub division of the base axial mesh

[2)] Eigenvalue error ($\Delta\rho$) from the corresponding MCNP reference solution (1.07777)

The fact that the decoupled scheme has comparable error with the coupled scheme means that once the radial heterogeneity effect is properly resolved with the planar MOC calculation, the axial heterogeneity effect can be resolved merely by the 3-D CMFD solution so that there is no need for performing planar MOC calculation with thin planes. This fact is confirmed by examining the variation of the generated homogenized cross section along the axial direction. As shown in Figure 2, the homogenized transport cross section obtained from the coupled calculation remains almost constant while the pseudo absorption cross section change relatively large. Thus it is reasonable not to perform the planar MOC calculation as long as the material composition is the same over several planes.

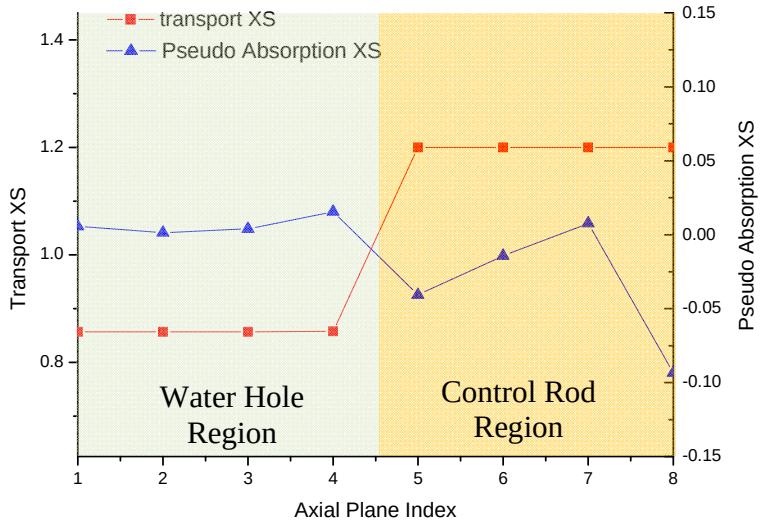

Figure 2. Variation of transport and pseudo absorption cross section for Rodded A

The Rodded Cases of A and B of the C5G7MOX benchmark problem are unrealistic ones in that the reflective condition is used at the bottom of the problem domain. In order to examine the decoupled scheme in a more realistic core, two rodded problems were created. It has the same radial configuration as the original rodded C5G7MOX problem. But it has longer axial domain consisting of nine 21.42 cm thick planes in the active core region. The zero incoming current condition is used in the bottom of the core. The 4 plane rodded problem shown in Table IV has the control rod inserted at four planes from the top of the active core. The 6 plane rodded problem is a more difficult problem because the control rod is inserted more than half of the active core resulting a significantly bottom skewed axial power distribution. Even for these more difficult rodded problems, the decoupled scheme works pretty well leading essentially the same accuracy as the coupled one as shown in Table IV.

Table IV. Comparison of Coupled and Decoupled Solutions for Modified Rodded Cases of C5G7MOX

Calculation Mode		Coupled		Decoupled	
Number of Rodded Plane		4	6	4	6
Eigenvalue Error, pcm[1)]		11	39	11	39
Axially Integrated Pin Power Error (%)	Maximum	4.76	1.83	4.88	2.05
	Mean	0.94	0.45	0.97	0.46
	RMS	1.26	0.51	1.84	0.56
Computing Time (sec)	RT	2063.6	2063.4	1067.5	1066.2
	CMFD	456.5	395.9	694.2	601.5

[1)]Eigenvalue error ($\Delta\rho$) from the corresponding MCNP reference solution (1.16112, 1.13329, respectively)

In Tables II and III, larger eigenvalue errors are noted for the coupled and decoupled cases as the axial mesh size becomes smaller. It turned out that in our previous work [6] that the increasing eigenvalue error is due to the use of the diffusion equation for the axial variation and this abnormal error behavior disappears with the SP3 solver in the axial direction. Based on the previous observation, it is expected that the decoupled scheme for the SP3 solver would have the same accuracy as the coupled scheme.

4. CONCLUSIONS

The decoupled planar MOC based 3-D CMFD scheme enables an approximate 3-D direct whole core transport calculation with the accuracy comparable to the coupled one. The computing time of the decoupled scheme can be effectively reduced because the planar MOC calculations can be selectively performed for the planes having different compositions. Since it was shown to be plausible to use the decoupled scheme even for the severely rodded C5G7MOX problems, this scheme can be applied to the realistic cases requiring thermal feedback without any signficant loss of accuracy. For the core calculation with thermal feedback, the group constants to be generated by each planar MOC problem should be given as a function of temperature. This functionalization of the group constants can be achieved by performing an additional planar MOC calculation at a higher power condition. The microscopic cross sections of each cell can then be represented as a linear function of temperature. This scheme of the decoupled calculation would increase the stability and the efficiency of the direct whole core calculation with thermal feedback.

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