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On the Diffusion Coefficient of Two-step Method for LWR analysis

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1. Introduction

The two-step method of the lattice transport calculation and the nodal diffusion calculation has been widely used in light water reactor (LWR) core analyses [1,2]. The two-step procedure consists of an assembly transport calculation with a lattice physics code, and a reactor core calculation with a nodal diffusion code. The few-group constants including diffusion coefficients are generated from the assembly calculation results.

Once the assembly calculation is done, the cross sections (XSs) are spatially homogenized, and a critical spectrum calculation is performed in order to take into account the neutron leakages of the lattice. The diffusion coefficient is also generated through the critical spectrum calculation. Three different methods of the critical spectrum calculation such as B_1 method [1,3], P_1 method [1], and fundamental mode (FM) calculation method [2] are considered in this paper. The diffusion coefficients can also be affected by transport approximations for the transport XS calculation which is used in the assembly transport lattice calculation in order to account for the anisotropic scattering effects. The outflow transport approximation [1] and the inflow transport approximation [4] are investigated in this paper.

The accuracy of the few group data especially the diffusion coefficients has been studied to optimize the combination of the transport correction methods and the critical spectrum calculation methods using the UNIST lattice physics code STREAM [4]. The combination of the inflow transport approximation and the FM method is shown to provide the highest accuracy in the LWR core calculations.

2. Diffusion Coefficient Calculation Method

Two factors are considered for the investigation of the accuracy of diffusion coefficients. The first one is the methods of critical spectrum calculation, B_1 method, P_1 method, or FM method. The second one is the transport correction methods, the outflow or the inflow transport approximations.

2.1 Critical Spectrum Calculation

In assembly lattice calculations, reflective boundary conditions are used assuming zero neutron leakage. However, the assemblies will be loaded in a reactor core with non-zero leakages. For the consistency between the homogenized XS generation from the lattice calculation and its use in the nodal diffusion analysis, the lattice physics code needs to take account of the neutron leakages at the assembly lattice calculation step. The leakage effects can be included by the critical spectrum calculation. The multi-group B_1 equations can be written as the following equations [1,3]

$$\Sigma_{t,g}\phi_g - \sum_{g'}\Sigma^0_{s,g'\to g}\phi_{g'} \pm iBJ_g = \chi_g \ , \qquad (1)$$

$$3a_g(B)\Sigma_{t,g}J_g - 3\sum_{g'}\Sigma^1_{s,g'\to g}J_{g'} = \mp iB\phi_g \, , \qquad (2)$$

where g is a multi-group index; $\Sigma_{t,g}$ is the total XS of group g; ϕ_g and J_g are the neutron flux and current; B is an energy independent buckling; χ_g is a fission spectrum; $\Sigma^0_{s,g'\to g}$ and $\Sigma^1_{s,g'\to g}$ are P_0 and P_1 scattering matrices, respectively; and, $a_g(B)$ is defined as follows

$$a_g(B) = \begin{cases} \frac{1}{3}x^2\left(\frac{\arctan(x)}{x-\arctan(x)}\right) & \text{for } x^2 = (B/\Sigma_{t,g})^2 > 0 \\ \frac{1}{3}x^2\left(\frac{\ln\left(\frac{1+x}{1-x}\right)}{\ln\left(\frac{1+x}{1-x}\right)-2x}\right) & \text{for } x^2 = -(B/\Sigma_{t,g})^2 > 0 \end{cases} . \qquad (3)$$

In the B_1 method, the critical buckling is searched in order to make the assembly critical. The flux solution from the B_1 method is used in condensing the multi-group zero-dimensional XSs into few-group (usually two-group) XSs. The diffusion coefficient is calculated as follows:

$$D_g = \frac{iJ_g}{|B|\phi_g} \ , \qquad (4)$$

where D_g is a multi-group diffusion coefficient of group g. The diffusion coefficient is then condensed to few-group (G) using the critical spectrum as follows:

$$D_G = \sum_{g\in G} D_g\phi_g \Big/ \sum_{g\in G}\phi_g \quad . \tag{5}$$

The P_1 method uses an identical procedure to the B_1 method except for the omit of $a_g(B)$ in Eq. (2) as follows:

$$3\Sigma_{t,g}J_g - 3\sum_{g'}\Sigma^1_{s,g'\to g}J_{g'} = \mp iB\phi_g \quad . \tag{6}$$

The solutions of Eqs. (1) and (6) with the critical buckling are used for the generation of diffusion coefficients by Eqs. (4) and (5).

On the other hand, in the FM method, the critical spectrum is calculated through the fundamental mode equation [2] as follows:

$$(\Sigma_{tr,g} - \Sigma^0_{s,g\to g})\phi_g + D_g B^2\phi_g = \chi_g + \sum_{g'\neq g}\Sigma^0_{s,g'\to g}\phi_{g'} \quad , \tag{7}$$

where $\Sigma_{tr,g}$ is a multi-group transport XS; and D_g is defined as follows using the transport cross section:

$$D_g = \frac{1}{3\Sigma_{tr,g}} \quad . \tag{8}$$

In the FM method, the P_1 scattering XS is not needed because the multi-group diffusion coefficients are calculated from the spatially homogenized transport XS. The critical spectrum is calculated from the buckling search, and used in the condensation to few-group constants including diffusion coefficients.

2.2 Transport Cross Section

The critical spectrum calculation is performed for fuel assemblies. For the reflector XSs, the solution of the lattice calculation with a fuel assembly and an attached reflector is directly used in the generation of few-group constants of the reflector without critical spectrum calculation. Since the transport XS affects the lattice calculation, the transport XS is one of the major factors affecting on the accuracy of diffusion coefficient. Furthermore, the diffusion coefficients depend on the transport XSs in the FM method because the diffusion coefficient is directly calculated from the multi-group transport XS, Eq. (8).

Two methods are considered for the transport XS generation. The outflow transport correction method [1] in Eq. (9) has been widely used in lattice physics codes.

$$\Sigma_{tr,g} = \Sigma_{t,g} - \sum_{g'}\Sigma^1_{s,g\to g'} \quad . \tag{9}$$

A more rigorous method, i.e., the inflow transport correction method can be written as follows:

$$\Sigma_{tr,g} = \Sigma_{t,g} - \frac{\sum_{g'=1}\Sigma^1_{s,g'\to g}\phi^1_{g'}}{\phi^1_g} \quad , \tag{10}$$

where ϕ^1_g is the P_1 flux moment. In the inflow transport approximation [4], the high order flux moment is calculated by solving one-dimensional P_N equation with moderator materials and approximated buckling. It was known that the outflow transport XS tends to overestimate neutron leakages, and it can cause large errors for high leakage problems [4].

3. Numerical Results

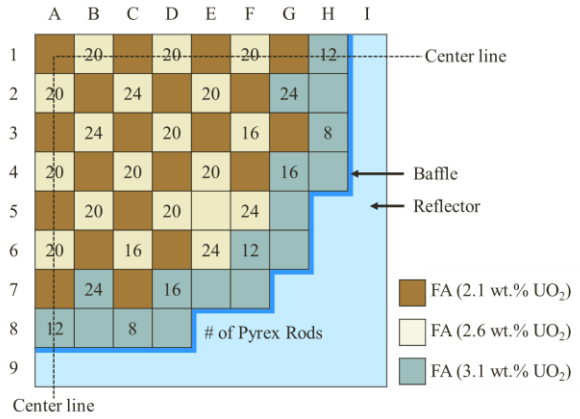

Fig. 1. Core loading pattern of test LWR problem [4].

A typical LWR problem in Fig. 1 [4] was selected for the comparison of methodologies on diffusion coefficients. Six calculation methods are selected as follows:

1) OB : Outflow transport XS+B_1 method.
2) OP : Outflow transport XS+P_1 method.
3) OF : Outflow transport XS+FM method.
4) IB : Inflow transport XS+B_1 method.
5) IP : Inflow transport XS+P_1 method.
6) IF : Inflow transport XS+FM method.

A lattice physics code STREAM [4,5] and nodal diffusion code PARCS [6] are used for the analyses of the six methods. In the lattice calculation, transport corrected P_0 calculation is performed with 70 energy groups. As results of the lattice calculation, discontinuity factors for fuel assembly and reflector are generated in order to reproduce the transport solution in the diffusion calculation [7].

The OB method is widely used in many reactor analysis codes [1], and the IF method is used in the STREAM code as a default. The two-group data are calculated for ten fuel assembly types using the six methods. In the reflector calculation, the adjacent fuel assembly is modeled together (2×1 color set). The number of 2×1 color sets is four (the reflectors facing FA with no Pyrex rod, 8 Pyrex rods, 12 Pyrex rods, and the reflector at the corner).

Table I: LWR core calculation results.

Method	k-eff	Diff. (pcm)	Assembly Power Diff. (%)		
			RMS.	Max.	Peak
MCNP6	1.00097	±1	±0.01	±0.01	±0.01
OB	1.00058	-39	0.76	1.79	0.81
OP	1.00039	-58	0.91	2.33	0.74
OF	0.99975	-122	2.36	4.70	-0.22
IB	1.00058	-39	0.89	2.00	0.83
IP	1.00039	-58	0.62	1.29	0.72
IF	1.00031	-66	0.57	1.28	0.53

1.0301 (0.005)	0.9541 (0.005)	1.0377 (0.005)	1.0148 (0.005)	1.1389 (0.005)	1.0606 (0.005)	1.0648 (0.005)	0.7677 (0.005)
0.9544 (0.005)	1.0219 (0.005)	0.9239 (0.005)	1.1001 (0.005)	1.0694 (0.005)	1.1616 (0.005)	1.0475 (0.005)	0.8764 (0.005)
1.0384 (0.005)	0.9242 (0.005)	1.0750 (0.005)	1.0522 (0.005)	1.1799 (0.005)	1.1462 (0.005)	1.0790 (0.005)	0.7759 (0.010)
1.0152 (0.005)	1.1006 (0.005)	1.0521 (0.005)	1.1742 (0.005)	1.1030 (0.005)	1.1458 (0.005)	1.0265 (0.005)	0.6290 (0.010)
1.1394 (0.005)	1.0698 (0.005)	1.1797 (0.005)	1.1029 (0.005)	1.3102 (0.005)	0.8993 (0.005)	0.9179 (0.005)	
1.0610 (0.005)	1.1617 (0.005)	1.1458 (0.005)	1.1457 (0.005)	0.8992 (0.005)	0.8993 (0.005)	0.6022 (0.010)	
1.0657 (0.005)	1.0479 (0.005)	1.0789 (0.005)	1.0262 (0.005)	0.9177 (0.005)	0.6020 (0.010)		
0.7684 (0.005)	0.8768 (0.005)	0.7758 (0.010)	0.6288 (0.010)			MCNP6 SD. [%]	

Fig. 2. Assembly power distribution and standard deviation of the reference MCNP6 results [4].

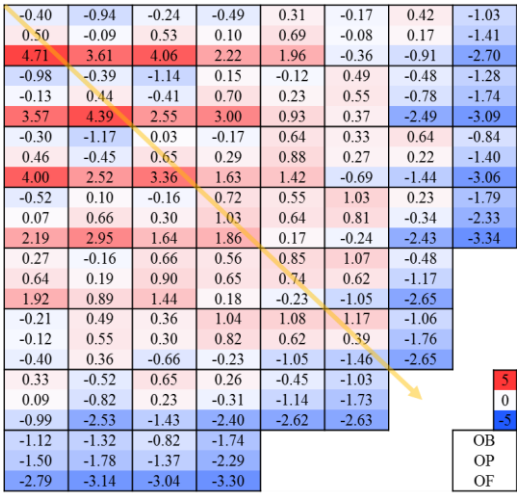

Fig. 3. Difference in assembly power distribution of OB, OP and OF methods (unit: %)

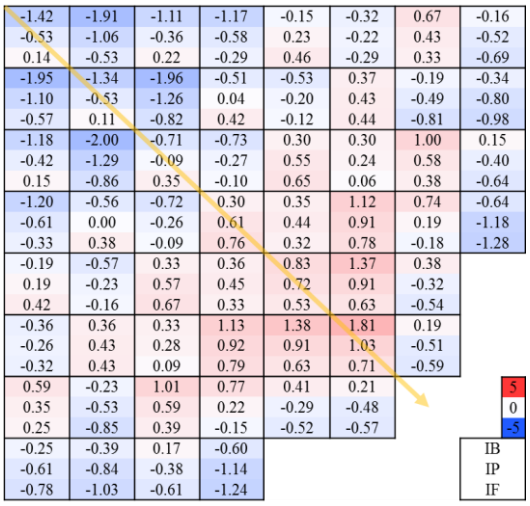

Fig. 4. Difference in assembly power distribution of IB, IP and IF methods (unit: %)

The results of the LWR core analyses are presented in Figs. 2, 3, 4, and Table I. MCNP6 [8] is used as a reference. In the six methods, the differences in k-eff are small. All the methods shows good agreement in k-eff compared to MCNP6 within the order of 100 pcm difference.

The OB method, which is adopted in many codes, shows accurate results of assembly power distribution. The RMS averaged difference is 0.76 % and the maximum difference is 2 %. There is a slight tilt of the assembly power distribution on the diagonal from -0.4 % to 1.17 %. The OP and OF methods show larger errors compared to the OB method. Especially, the OF method shows significant tilts in power distribution from 4.71 % to -1.46 %.

With the inflow transport correction, the overall assembly power distributions become more accurate except for the method IB. The inflow based methods (IB, IP and IF) show different trends than the outflow based methods (OB, OP and OF). In the outflow correction based method, the FM method shows the largest errors, and the B_1 method shows the smallest errors. The tendency is opposite in the inflow correction based methods. The IF method shows the most accurate results among the six methods. The RMS difference is as low as 0.57 % and the maximum difference is 1.28 %. The IF method shows 1.3 ~ 1.4 times improved accuracy of the assembly power distribution compared to the conventional method (OB). The IF method also greatly reduces the tilt of power distribution. The IF method shows 0.14 % to 0.71 % along the assemblies on the diagonal.

The diffusion coefficient is a major factor causing the differences in power distributions. Figs. 5 and 6 show the comparison of two-group constants of an assembly in the position (1, B) and a reflector in the position (2, I), respectively. The two-group constants from the IF method is considered as a reference as in Table II.

There is no significant difference in the absorption, fission XSs, and assembly discontinuity factors for fuel assemblies. For the assembly calculation, the critical spectrum calculation method is more important rather than the transport XS except for the OF method because the diffusion coefficient of the OF method is directly calculated from the transport XS. The method OB and IB shows similar diffusion coefficients each other, and the methods OP and IP show similar results. Because the critical spectrum calculation is not performed for reflectors, the two-group constants of reflectors are calculated with the transport XSs and infinite spectrum. Therefore there is no difference between inflow based methods in Fig. 6.

Table II: Two-group constants from IF method.

Group [1], Position	D [2] (cm)	Abs [3] (cm^{-1})	Fis [4] (cm^{-1})	DF [5] (-)
G_1, (1,B)	1.39246	0.01000	0.00607	1.00994
G_2, (1,B)	0.39882	0.09934	0.11503	1.11652
G_1, (2,I)	1.24758	0.00256	-	1.21087
G_2, (2,I)	0.27839	0.04220	-	0.27362

1) $G_1$is fast group; and G_2 is thermal group. 2) Diffusion coefficient.
3) Absorption XS. 4) Fission XS.
5) Assembly discontinuity factor for fuel assembly (1,B), and discontinuity factor for reflector (2,I).

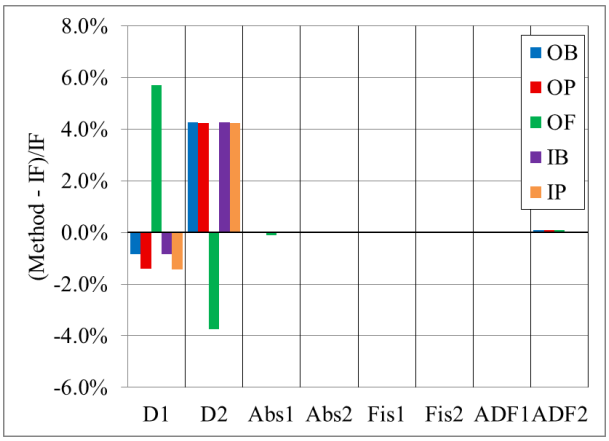

Fig. 5. Comparison of two-group constants of fuel assembly in position (1, B).

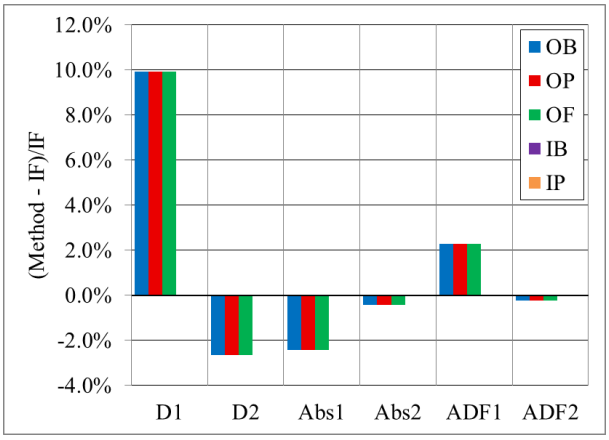

Fig. 6. Comparison of two-group constant of reflector in position (2, I).

4. Conclusions

The methodologies to calculate the diffusion coefficients have been reviewed, and the performances of them have been investigated with a LWR core problem. The combination of the inflow transport approximation and the fundamental mode critical spectrum calculation shows the smallest errors in terms of assembly power distribution. There is no meaningful difference in the multiplication factors of different methods for the tested LWR core problem. The test results shed lights on how to calculate the diffusion coefficients accurately for the two-step method applied to LWRs.

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