Nodal Equivalence Theory Based on Functionalized Discontinuity Factors

Woosong Kim and Yonghee Kim*

Dept. of Nuclear and Quantum Eng., KAIST, 373-1 Daehak-ro, Yuseong-gu, Daejeon, Korea, 305-701 *Corresponding author: yongheekim@kaist.ac.kr

1. Introduction

The contemporary reactor core analysis for the Light Water Reactor (LWR) heavily replies on the fuel assembly homogenization based on the nodal equivalence theory, which is the idea of preserving the equivalency between an original heterogeneous assembly and a homogenized assembly in terms of reaction rates and node interface currents [1]. In the nodal equivalence theory, the single assembly homogenization is most widely used to obtain homogenized parameters for the calculational efficiency. However, because reflective boundary conditions are used for the single assembly calculation, the accuracy of whole core analysis deteriorates noticeably when two very different assemblies are neighboring each other and the node interface current is not close to zero [2]. In this study, we propose a new and unique approach to reduce the error which comes from the incomplete assembly homogenization in the lattice calculation.

2. Functionalized Discontinuity Factors

Because the conventional assembly discontinuity factors (ADFs) are based on the net-zero current boundary condition, they may be quite different from the reference Discontinuity Factors (DFs) which are obtained by using the exact boundary conditions. However, if one can generate the DFs as a function of boundary condition of a fuel assembly in the lattice calculation and the DF can be updated by using the actual current information during the iterative core calculation, it is expected that more accurate DFs will determined and the resulting nodal equivalence for the homogenized fuel assemblies will improved, leading to a more accurate core analysis. This conjecture is based on the general perception that the interface neutron current from a core calculation should be 'closer to the reference' than the 'zero net-current' conditions used for determination of the conventional ADFs. If the perception is true, update of DFs by using the 'more accurate' interface current resulting from the whole core calculation will provide correspondingly 'improved DFs' to be used in the next iterative core calculation and the accuracy of the resulting core calculation could be improved again and the DF updated follows. In this way, the non-linear DF update can be continued until convergence. In a sense, the associated algorithm is based on a 'virtuous cycle' between the DFs and interface currents. To see the feasibility of the

functionalized discontinuity factors (FDFs), onedimensional test problems are considered in the work.

2.1. Functionalization of discontinuity factor

In this study, we tried to functionalize DFs of a surface by using the current-to-flux ratio (CFR) on the same surface only because the surface DFs are mainly dependent on the surface boundary condition for the same surface. Of course, DF may also depend on the boundary conditions on the other surfaces of the fuel assembly. However, in this work, the FDF is assumed to depend only on the CFR of the same surface for practical and efficient applications of the FDF concept. Figure 1 shows the schematic illustration of the FDF in a 1-D fuel assembly geometry.





The FDFs are expressed as a function of node interface CFR. For the functionalization of FDFs, either linear or quadratic functions are used in this study:

$$DF_g^L = ADF_g \left[a_1 + a_2 \left(\frac{J_g^L}{\phi_g^L} \right) \right], \tag{1}$$

$$DF_g^L = ADF_g \left[a_1 + a_2 \left(\frac{J_g^L}{\phi_g^L} \right) + a_3 \left(\frac{J_g^L}{\phi_g^L} \right)^2 \right], \quad (2)$$

where DF_g^L is the g-th group DFs on the left surface of a homogenized assembly, ADF_g is the conventional gth group assembly discontinuity factor, a_n are coefficients, ϕ_g^L is the flux on the left surface of heterogeneous assembly, and J_g^L is the current on the left surface of heterogeneous assembly. The DFs on the right surface is also functionalized in the same way.

In order to determine the coefficients a_n , the 1-D lattice problem in Fig. 1 is solved by using several CFR boundary conditions on each surface. Because the CFR is a function of albedo in diffusion approximation, a set of albedo boundary condition was used for the set of CFR boundary conditions. The CFR boundary condition can be either positive or negative in actual problems. Therefore, 3 CFR (+, 0, -) boundary conditions are used

on each surface in this work, and 1-D lattice problem is solved 3 times with different boundary conditions, instead of the single fuel assembly analysis in the conventional method. It is worthwhile to note that, in the case of symmetric fuel assembly, the FDF is identical for all surfaces if a single set of CFR values is used for the FDF determination. As a result, the number of fuel assembly analysis is only increased from 1 to 3 even in a 2-D fuel assembly problem. In addition to the conventional zero CFR, 2 CFRs are additionally used for determination of the FDF. Thus, in the case of the linear FDF, the 2 coefficients should be determined in a least square sense.

Unlike the symmetric fuel assembly analysis, in the case of heterogeneous baffle-reflector homogenization, a set of current boundary conditions are used instead of albedo boundary condition to determine the homogenized parameters and the coefficients for FDF. As shown in Fig. 2, just like in the conventional bafflereflector homogenization, a small spectral fuel-reflector model is analyzed. The heterogeneous current at the interface from the spectral geometry is used as reference value. Similarly to the fuel assembly calculation, 3 current (+ ε , reference, - ε) boundary conditions are used on the reflector surface to determine the FDF coefficients. Of course, one of the current information is from the fuel-reflector spectral analysis and the other two conditions are determined appropriately. For the reflector nodes, both linear and quadratic FDFs are applied, as well.



Fig. 2. The heterogeneous reflector FDF evaluation

2.2. Whole-core calculation with FDFs

In the whole-core analysis based on the welldeveloped inner-outer nested iterations, the FDFs are updated by using the node interface CFR during iteration (FDF iteration). The lattice or fuel assembly calculations with different CFR boundary conditions provides different homogenized group constants for the fuel assembly. However, in the work, the other homogenized parameters, such as diffusion coefficients and cross-sections are fixed to the conventional fluxweighted constants (FWCs) determined with zero CFR boundary condition [3].

Fig. 3 shows the iterative solution scheme including an FDF update iteration. In Fig. 3, t is index of "outer iteration" and u is index of "FDF iteration", the update procedure for DFs in Eqs. (1) and (2). During above iterations, different error criteria was used to check the convergence of outer iteration and FDF iteration.



Fig. 3. Flowchart of the FDF iterative solution scheme

3. Results and Discussion

Two one-dimensional slab geometry problems were considered to test the above-mentioned FDF method. The reflective boundary condition is imposed on the left hand side and the right hand side is subject to the vacuum boundary condition.

3.1. UO₂ fuel loaded 1-D core problem

As shown in Fig. 4, in the first test problem, there are 10 fuel assemblies in the core region and two types of UO_2 fuels are loaded; Fuel 1 and Fuel 2 with slightly different enrichment. The length of a fuel assembly is 22.8 cm and control rods are inserted into 5 fuel assemblies in the core. The fuel assembly is comprised

of fuel, coolant, and water. It is assumed that 2-group cross sections are provided for each material in the test problem.

ŀ	22.8 cm ⁺ 22.8 cm ⁺	2.4 cm ¹ 20.4 cm
	🔄 Fuel 1 📃 Fuel 2 🔲 Control rod 🗌 Water 📕 Baffle	

Fig. 4. Configuration of test problem I

The main objective of this study is to see the feasibility of the FDF method. For the analysis of the fuel assembly and core, a 1-D diffusion finite difference method (FDM) code was developed for both whole core and lattice calculations. A very fine mesh (0.01 cm) was used in the analysis and the error criteria between FDF iteration steps were $\varepsilon_{keff} < 10^{-7}$ for the multiplication factor and $\varepsilon_{source} < 10^{-6}$ for the source distribution.

First, each fuel assembly and the baffle-reflector were homogenized with CFR=0 condition and 2 additional analyses were performed to determine the FDF for each type of fuel assemblies and baffle-reflector. Figure 5 shows the resulting FDFs of an assembly type in the problem. From Fig. 5, it is clear that the FDF is rather non-linear function of the CFR boundary condition for both thermal and fast groups. Also, Fig. 5 shows that the thermal FDFs are closer to unity than fast FDFs, as expected.



Fig. 5. The DF as a function of current-to-flux ratio

During FDF iterations, the FDFs were updated whenever outer iteration satisfies the error criteria which is 10 times looser than that of FDF iteration. Consequently, the FDF update is triggered only when the fission source is roughly converged.

Table I compares the effective multiplication factors of each solution scheme with the reference value. It is observed that the conventional ADF provides an improved k_{eff} than without any DFs. One can also clearly notes that, when the liner FDF in Eq. (1) is used, the k_{eff} error is reduced by only about 15% in comparison to the

conventional simplified equivalence theory (SET) with ADFs. However, the quadratic FDF of Eq. (2) provides a much improved result, which shows about 65% reduced error compared with the SET result.

Table I. The effective multiplication factor comparison (test problem I)

	$k_{e\!f\!f}$	Error	# of outer
		(pcm)	iteration
Reference	0.853100	-	446
w/o DF	0.847584	-552	443
ADF	0.850986	-211	438
FDF(linear)	0.851304	-180	469
FDF(quadratic)	0.852369	-73	470

From Table I, it also is noticeable that the total number of outer iterations increases only slightly from the SET case, which means that the FDFs converges quickly and the computing time of whole-core calculation with FDFs will be comparable to the conventional method. The k_{eff} convergence behavior is shown in Fig. 6. It is important to note in Fig. 6 that the 1st update of FDFs improves the k_{eff} value a lot and the successive FDF updates lead only to a marginal additional improvement. It is expected that only a few updates of the FDF will provide sufficiently improved accuracy of the solution. In the FDF iteration, it was observed that the FDF update may experience an over correction and the overall convergence can be impaired. However, it was found that over-correction of FDF can be easily fixed by using an under-relaxation of the FDF update.



Fig. 6. The keff value vs. outer iteration in test problem I

Figure 7 shows the assembly-wise normalized power distribution for each method and Table II shows the error in the assembly power profile. As shown in Table II, the maximum relative error and RMS error decreased a lot for both FDF schemes. Nevertheless, the absolute error of the quadratic FDS is rather high due to the extremely distorted power distribution caused by the heavy control rod insertion.



Fig. 7. Assembly power distribution (test problem I)

	Max. relative	RMS
	error (%)	error (%)
w/o DF	9.150	4.169
ADF	7.162	2.834
FDF(linear)	0.965	0.499
FDF(quadratic)	3.334	1.508

Table II. Power distribution comparison (test problem I)

3.2. UO2 and MOX fuel loaded 1-D core problem

A modified problem was also tested in which assemblies 4 and 8 are replaced with Fuel 3, which is a MOX fuel. The configuration of the second test problem is shown in Fig. 8.

1						Bane	
1	22.8 cm 22.8 cm	∲•∳	*****	*****	•/• •	2.4 cm ³ 2	0.4 cm
	E Fuel 1	Fuel 2	Fuel 3	Control rod	Water	Baffle]

Fig. 8. The configuration of test problem II

Because the neutronic characteristics of the MOX fuel is significantly different from the UO_2 fuel, it is known that the application of nodal equivalence theory are more difficult for the MOX-containing problem. The results for the MOX-UO₂ core are summarized in Table III.

Table III. The effective multiplication factor comparison (test problem II)

	k _{eff}	Error	# of outer
	-33	(pcm)	iteration
Reference	0.868007	-	643
w/o DF	0.860645	-736	608
ADF	0.865856	-215	630
FDF(linear)	0.865980	-203	616
FDF(quadratic)	0.866993	-101	602

When the MOX fuel is loaded into the core, the linear FDF just marginally improves the accuracy of k_{eff} . However, it is clearly noted that the quadratic FDF still provides a much improved k_{eff} value, reducing the k_{eff} error by about 53%. From Table III, it is also interesting to note that the number of outer iterations in the FDF case is even slightly reduced than in the conventional SET method.

The convergence behavior of k_{eff} is shown in Fig. 9 for the 2nd problem. In this case, the FDF update begin after ~400 outer iterations. Similarly to the problem I case, one can observe that the k_{eff} error is reduced noticeably after the 1st and/or 2nd FDF update and the continued updates provides a small improvement as in the 1st test problem.



Fig. 9. The k_{eff} value vs. outer iteration (test problem II)

Figure 10 shows the normalized assembly power distribution of the test problem II and Table IV shows the errors in the power profiles.



As shown in Table IV, it is clear that the quadratic FDF can improve the assembly power distribution in the difficult MOX-containing core problem. The maximum

relative error was decreased by ~51% for the 2^{nd} order FDF, and RMS error was also decreased by ~36% for the 2^{nd} order FDF.

Table IV. Power distribution comparison (test problem II)

	Max. relative	RMS
	error (%)	error (%)
w/o DF	11.750	5.830
ADF	4.293	1.796
FDF(linear)	2.243	1.065
FDF(quadratic)	2.089	1.158

4. Conclusions

In this study, we have proposed a new and unique method to improve accuracy of the nodal equivalence theory in reactor core analysis. The DFs are expressed as a function of node interface current-to-flux ratio. The evaluation of FDFs requires just a few more lattice calculations and they are updated during iterative calculation of whole-core calculation without significant change in computing time. It is clearly demonstrated that a quadratic FDFs can reduce the k_{eff} error more than 50% in both conventional UO₂ and UO₂-MOX problems. Also, we have shown that the assembly power distribution is improved by using the FDF method. For a more practical utilization of the FDF method, its feasibility study for two-dimensional practical fuel assembly problems is underway.

REFERENCES

[1] K. S. Smith, "Assembly Homogenization Techniques for Light Water Reactor Analysis," *Progress in Nuclear Energy*, 17, 303 (1986).

[2] K. T. Clarno and M. L. Adams, "Capturing the Effect of Unlike Neighbors in Single-Assembly Calculations," *Nucl. Sci. Eng.*, Vol. 149, p. 182 (2005).

[3] A. F. Henry, *Nuclear-Reactor Analysis*, The MIT Press, Cambridge, Massachusetts (1975).