Importance of Assembly Discontinuity Factors In Simulating Reactor Cores Containing Highly Heterogeneous Fuel Assemblies

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Abstract: To assess the importance of assembly discontinuity factors (ADF), a highly heterogeneous reactor core was simulated using a COMSOL model in which ADF are not used. The resulting errors in assembly powers were found to be unacceptably high. This indicates that for highly heterogeneous cores such as one with MOX and LEU fuel assemblies, the use of techniques that counter the effect of homogenization, such as ADF, are necessary to reduce power errors to acceptable levels. A direct correlation was found between ADF and assembly power error.

Keywords: General Equivalence Theory (GET), Assembly Discontinuity Factor (ADF), two-energy-group neutron diffusion equation, PDE Coefficient Form Eigenvalue mode.

1. Introduction

Most modern reactor core physics codes rely on a solution of the few-group neutron diffusion equation. To make the computational time manageable, domains over which the equation is solved are often homogenized as much as possible, typically at the fuel assembly or lattice cell level. Because homogenization affects the solution, various techniques have been developed to counter the effect of homogenization. One technique is through the use of what is now commonly known as assembly discontinuity factors (ADF) [1].

In reactor cores where the lattice design results in a low degree of heterogeneity, such as in a CANDU® Reactor, the use of ADFs is less important and can usually be ignored [2]. However, this may not be the case in reactors that use light water as a moderator/coolant, and with reactors that use a mix of lattices with low enriched uranium (LEU) and mixed uranium/plutonium oxide (MOX) fuels.

This paper reports the results of studies performed to examine errors in assembly powers when ADF's are not implemented in the analysis of a relatively heterogeneous reactor core, making use of data from an international benchmark problem [3]. The purpose of the benchmark problem was to assess the ability of modern reactor physics codes, which use ADFs, to simulate the utilization of weapons-grade plutonium in a four-loop Westinghouse (Pressurized Water Reactor) PWR.

A complete information package was obtained for the international benchmark problem from the NEA [4], which contained all input parameters, the geometry as well as output from various participants in the benchmark study of a Westinghouse PWR loaded with MOX and LEU fuel assemblies.

The core chosen for the benchmark simulation was based on a four-loop Westinghouse PWR power plant similar to the reactor chosen for plutonium disposition in the USA. COMSOL [5], a finite element package was used to solve the two-group neutron diffusion equation using the built-in PDE Coefficient Form Eigenvalue mode.

The information package ensured that data used in the COMSOL simulation was identical to that used in the benchmark study. Due to the complexity of the geometry and structure of the data files, the coupling of COMSOL and MATLAB [6] was essential. MATLAB was also used to automate the COMSOL simulation, for post-processing and comparing the COMSOL results with those from the other codes.

2. Theory and Analysis

The first step in the analysis was to create the geometry for the benchmark problem. The core consists of square fuel assemblies surrounded by a reflector with the same width as the fuel assembly pitch, as shown in Fig. 1.

Though COMSOL contains a CAD environment which allows creation of objects in 1-D, 2-D, and 3-D, it is often desirable to import a geometry that has been created in another CAD environment. In this case Solid Edge was used to create the geometry.

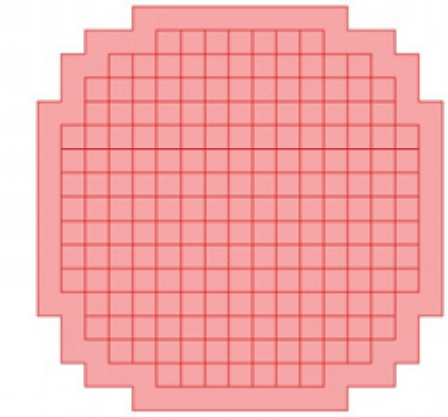

Fig. 1. Benchmark geometry

The mathematical problem being solved is the two-energy-group isotropic neutron diffusion equation.

$$-D_1\nabla^2\phi_1+\Sigma_{R1}\phi_1=\frac{1}{k_{eff}}\left[\nu\Sigma_{f1}\phi_1+\nu\Sigma_{f2}\phi_2\right]+\Sigma_{S21}\phi_2 \quad (1)$$

$$-D_2\nabla^2\phi_2+\Sigma_{R2}\phi_2=\Sigma_{s12}\phi_1 \quad (2)$$

where the removal cross sections are defined as

$$\Sigma_{R1}=\Sigma_{a1}+\Sigma_{s12} \quad (3)$$

$$\Sigma_{R2}=\Sigma_{a2}+\Sigma_{s21} \quad (4)$$

In the equations, numerical indices 1 and 2 designate fast and thermal neutrons or energy groups one and two respectively. The subscript 12 designates scatter from group 1 to 2 (downscatter) and 21 designates scatter from group 2 to 1 (upscatter) and the isotropic diffusion coefficient, $D = 1/(3\Sigma_{tr})$.

The right-hand sides of Eq. (1) and Eq. (2) are the source terms for each group, which are a result of fission and/or scatter from one group to another. It is assumed that all fission neutrons are fast neutrons.

The only source term for thermal neutrons is via downscatter from group 1. The left side of Eq. (1) Eq. (2) are the loss terms for each group, which occur as a result of leakage, absorption and scatter from one group to another.

Eq. (1) and Eq. (2) can be written in matrix notation as follows

$$\begin{pmatrix}-D_1\nabla^2+\Sigma_{R1} & -\Sigma_{S21}\\ -\Sigma_{S12} & -D_2\nabla^2+\Sigma_{R2}\end{pmatrix}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}=\frac{1}{k_{eff}}\begin{pmatrix}\nu\Sigma_{f1} & \nu\Sigma_{f2}\\ 0 & 0\end{pmatrix}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} \quad (5)$$

Eq. 5 is a generalized eigenvalue equation of the form

$$M\phi=\lambda F\phi \quad (6)$$

where M is the loss matrix given by scattering, leakage and absorption:

$$\begin{pmatrix}-D_1\nabla^2+\Sigma_{R1} & -\Sigma_{S21}\\ -\Sigma_{S12} & -D_2\nabla^2+\Sigma_{R2}\end{pmatrix}$$

F is the production term matrix given by

$$\begin{pmatrix}\nu\Sigma_{f1} & \nu\Sigma_{f2}\\ 0 & 0\end{pmatrix}$$

and the eigenvalue is

$$\lambda=\frac{1}{k_{eff}}$$

Eq. 5 is solved using COMSOL's built-in PDE Coefficient Form Eigenvalue mode, which has the form

$$\nabla\cdot(-c\nabla u-\alpha u+\gamma)+au+\beta\cdot\nabla u=d_a\lambda u-e_a\lambda^2 u \quad (7)$$

This can be made equivalent to Eq. 7 by setting

$$c=\begin{pmatrix}-D_1 & 0\\ 0 & -D_2\end{pmatrix}$$

and

$$\alpha=\begin{pmatrix}\Sigma_{R1} & -\Sigma_{S21}\\ -\Sigma_{S12} & \Sigma_{R2}\end{pmatrix}$$

and

$$d_a=\begin{pmatrix}\nu\Sigma_{f1} & \nu\Sigma_{f2}\\ 0 & 0\end{pmatrix}$$

Fig. 2 shows the fueling arrangement, which is a quarter-core loading pattern.

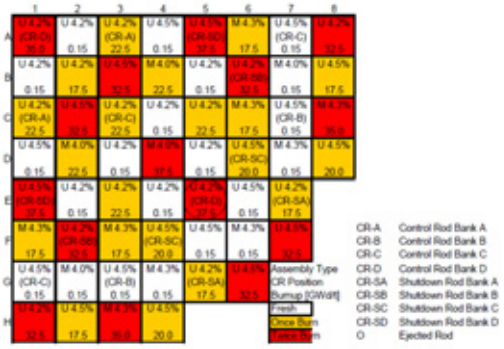

Fig. 2. Benchmark fuel loading scheme

M and U stand for MOX and Uranium fuels respectively, with enrichment (%) indicated beside the fuel designation. For each fuel type, the benchmark information package contains one data file covering a range of burnups. The full core geometry, shown in Fig. 1, is obtained by a series of reflections.

The last step in building this model is the selection of appropriate boundary conditions. Continuous flux and current interface boundary conditions, the default for interior surfaces, were

applied to all fuel assemblies and the inner reflector surface.

For the four outer reflector surfaces, a boundary condition derived from transport theory should be applied. This condition states that the flux is assumed to drop linearly outside the external reflector boundary and vanish at a distance of $0.7104\lambda_{tr}$. Fig. 3 illustrates the vanishing flux boundary condition in 1-D.

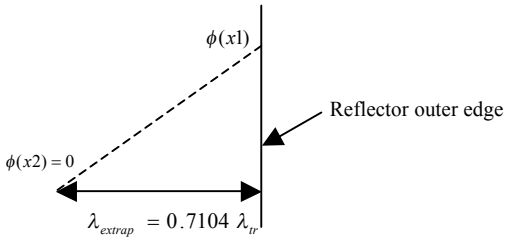

Fig. 3 Vanishing flux boundary condition

This can be reformulated as a boundary condition.

$$\left.\frac{d\phi}{dx}\right|_{x1} = \frac{\phi(x2)-\phi(x1)}{x2-x1} = \frac{-\phi(x1)}{x2} \qquad (8)$$

Substituting for x2, the expression for the boundary condition becomes

$$\left.\frac{d\phi}{dx}\right|_{x1} = \frac{-\phi(x1)}{0.7104*\lambda_{tr,g}} = \frac{-\phi(x1)}{2.1312*D_g} \qquad (9)$$

Generalizing to a multidimensional surface

$$\phi_b = -2.1312*D_g*\nabla\phi\big|_b \qquad (10)$$

where the subscript "b" designates the reflector vacuum boundary and D_g is the diffusion coefficient in the reflector for neutrons belonging to energy group g.

A Dirichlet boundary condition is of the form $h\phi = r$ where h, which in this particular problem is 1 and $r = -2.312* Dg * \nabla\phi|_b$. Unfortunately, the current implementation of the Dirichlet boundary condition in COMSOL does not permit a value of r other than 0. As a result, the COMSOL model in this analysis used a zero flux boundary condition at the outer edge of the reflector.

In reality, for most cores the flux vanishes at a distance of distance of 2-3 cm outside the reflector. It is therefore expected that the COMSOL model will return slightly higher errors for assembly powers adjacent to the reflector.

The Direct (PARDISO out of core) solver was chosen as it is a highly efficient solver for symmetric systems and often uses less memory than other solvers. The mesh used in the analysis is shown in Fig. 4, with rectangular mesh elements chosen for fuel assemblies.

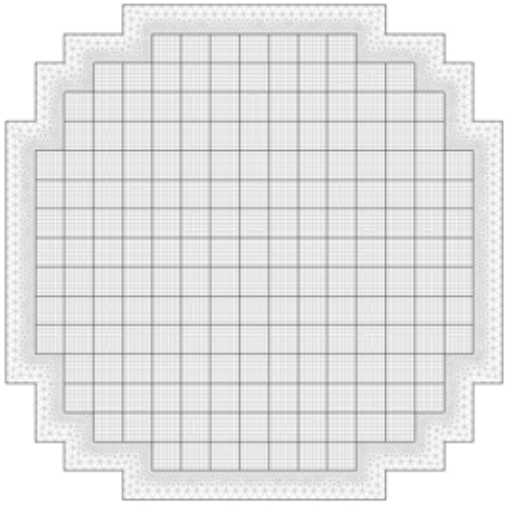

Fig. 4. Mesh used in COMSOL model

The parts of the benchmark problem analyzed were assembly powers and k_{eff} for the All Rods Out (ARO) state.

Each assembly (square region) shown in Fig. 1 actually consists of a 17x17 array of fuel pin cells, with each fuel pin in turn composed of concentric regions of water and fuel. Since modeling the detailed geometry at the pin and sub-pin level, called a heterogeneous model, is computationally expensive, most reactor physics codes often model the assemblies as a single unit, called a homogeneous model. Material and neutronic properties for the composite unit are obtained from homogenization of the assembly substructure.

Though computationally convenient, homogenization introduces errors when compared to a calculation which models fine details of the core. The principal error is in the node-integrated reaction rate in the assembly. An improvement to standard homogenization, widely used for light water reactors is Generalized Equivalence Theory (GET) [1]. According to GET the node-integrated reaction rates of the fine and coarse models can be matched by allowing for discontinuities in the surface multigroup flux at assembly boundaries. This is accomplished by a suitable multiplier for

the neutron flux on each side of a surface, called an assembly discontinuity factor (ADF).

The assembly discontinuity factor f is defined as the face-averaged flux heterogeneous flux $\overline{\psi}$, to the face-averaged homogeneous flux $\overline{\phi}$:

$$f = \frac{\overline{\psi}}{\overline{\phi}} \tag{11}$$

The discontinuity condition at the face between neighboring assemblies is written:

$$\overline{\phi^+} f^+ = \overline{\phi^-} f^- \tag{12}$$

where $\overline{\phi^+}$ is the face-averaged flux on one side of the surface and $\overline{\phi^-}$ is thee face-averaged flux on the other side; f^+ and f^- are the corresponding discontinuity factors.

It can be seen from Eq. 12, that:

$$\overline{\phi^+} = \overline{\phi^-} \frac{f^-}{f^+} \tag{13}$$

namely that the face-averaged flux in neighboring assemblies is dependent on the ratio of the respective assembly discontinuity factors.

As a result of the imposition of boundary conditions, the flux at the assembly boundaries will affect the flux distribution inside the assembly. It can therefore be expected that in highly heterogeneous cores, where the ratio of neighboring discontinuity factors deviates significantly from 1, homogenized reaction rates will differ from reaction rates using a detailed or heterogeneous model.

A metric used to gauge the effect of ADF on assembly fuel power is the average ratio of ADF on all four sides of a fuel assembly to that of its neighbors:

$$\overline{ADFR}_{(i,j)} = \frac{(ADF_{(i-1,j)} + ADF_{(i,j+1)} + ADF_{(i+1,j)} + ADF_{(i,j-1)})}{4ADF_{(i,j)}} \tag{14}$$

where i and j designate row and column respectively. Moreover since the energy release from thermal fission is very much greater than the energy release from fast fission, one would expect the correlation between $\overline{ADFR}_{(i,j)}$ and power error to hold only for thermal ADF. Assembly power in the COMSOL model was computed as

$$\frac{\iint_{bundle} (\kappa\Sigma_{f1}\phi_1 + \kappa\Sigma_{f2}\phi_2)}{\overline{\iint_{core} (\kappa\Sigma_{f1}\phi_1 + \kappa\Sigma_{f2}\phi_2)}} \tag{15}$$

The normalization factor in the denominator of Eq. 15, $\overline{\iint_{core} (\kappa\Sigma_{f1}\phi_1 + \kappa\Sigma_{f2}\phi_2)}$, which is the average power in the core, means that the average assembly power is 1.

3. Results and Interpretation

To assess the importance of assembly discontinuity factors, they were not used in the COMSOL model. The results were compared with those from the benchmark reference, DeCART [7], PARCS [8] with ADF and with PARCS with the ADF option turned off.

In order to accurately describe error distribution, two metrics are used for comparison of the results; the power-weighted error (PWE) and the error-weighted error (EWE). They are defined by Eq. (16) and Eq. (17) respectively

$$PWE = \frac{\sum_i |e_i| ref_i}{\sum_i ref_i} \tag{16}$$

$$EWE = \frac{\sum_i |e_i| |e_i|}{\sum_i |e_i|} \tag{17}$$

where

$$e_i = \frac{calc_i - ref_i}{ref_i} \tag{18}$$

and where $calc_i$ designates an assembly power for either COMSOL or PARCS and ref_i designates the corresponding reference assembly power from DeCART.

The PWE diminishes the importance of the error in the low power region and amplifies the importance in the high power region. The EWE is not linked to the power distribution but only to the magnitude of the error and can therefore magnify the effect of large errors in low power regions.

The results are shown in Table 1. Fig. 5 and Fig. 6 show the assembly power error distribution for COMSOL and PARCS with the ADF option turned off, respectively. Power errors of this magnitude are generally considered unacceptably high.

Fig. 7 shows the assembly power error distribution for PARCS when ADF are used. The errors are fairly small in magnitude, as indicated by the small PWE and EWE and are considered acceptable.

Table 1. Eigenvalue and assembly power comparison

Code	k_{eff}	Δ mk	%PWE	%EWE
DeCART	1.05852	ref	ref	ref
PARCS with ADF	1.06379	5.27	0.96	1.63
PARCS without ADF	1.06501	6.49	4.33	3.99
COMSOL	1.06500	6.48	3.76	11.0

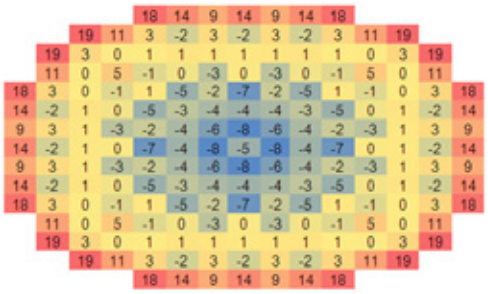

Fig. 5. Assembly power errors (%) - COMSOL with no ADF

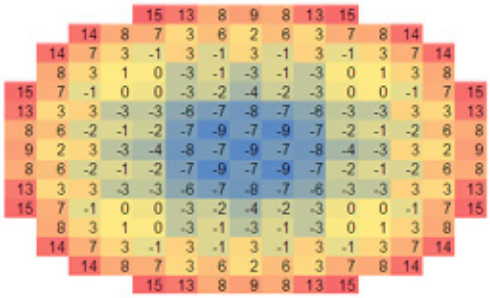

Fig. 6. Assembly power errors (%) - PARCS with no ADF

Fig. 8 shows the distribution of the average ADF ratio from 1. It can be seen that this ratio is highest for peripheral assemblies, which border the reflector. Fig. 9 is a plot of the COMSOL assembly power error versus $(\overline{ADFR}-1)*100$. The two quantities are well correlated, with a correlation coefficient of 0.9292.

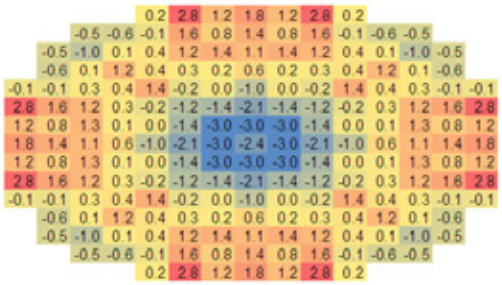

Fig. 7. Assembly power errors (%) – PARCS with ADF

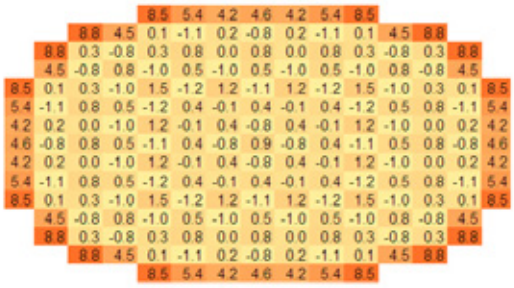

Fig. 8. Distribution of $(\overline{ADFR}-1)*100$

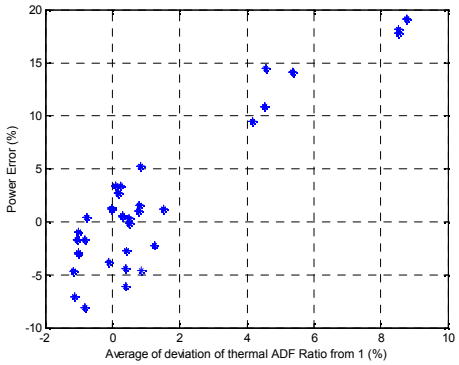

Fig. 9. Plot of COMSOL assembly power error (%) versus $(\overline{ADFR}-1)*100$

The k_{eff}, appears not to be affected much by ADF, with an error of less than 1 mk. Noteworthy is the fact that the k_{eff}, from COMSOL and PARCS with no ADF are almost identical, with a difference of only 0.01 mk.

4. Conclusions

For highly heterogeneous cores such as one with MOX and LEU fuel assemblies, the use of techniques that counter the effect of the homogenization, such as ADF, is necessary to reduce power errors to acceptable levels.

5. References

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