Abstract

JIANG, QUNLEI. Intra-nodal Study for the Mixed LEU-MOX Cores. (Under the direction of Paul J. Turinsky and Dmitriy Y. Anistratov).

One favored method being considered for the disposal of surplus weapons grade plutonium (WGPu) is to burn the WGPu as mixed oxide (MOX) fuel in commercial existing Light Water Reactors (LWRs). Duke Power Company intends to irradiate MOX fuel assemblies in their four Westinghouse pressurized water reactors (PWR). The introduction of MOX fuel into LWRs poses several challenges for the reactor physics analysis.

The difference in properties of uranium and plutonium induces neutron energy spectrum difference between the MOX and LEU assemblies, which creates a large thermal flux gradient at the interface between these assemblies. Current methods for predicting the intra-nodal flux distribution have difficulty to model this gradient.

This study is focused on improving the fidelity of the core simulator utilized in FORMOSA-P to model mixed LEU-MOX cores. In particular, the nature of challenge in regard to accurately model the LEU-MOX interfaces due to both strong spatial variations of the thermal flux and energy spectra, the later impacting the two-group cross section values, will be assessed. The specific focus is on pin-wise power reconstruction; however, issues related to the nodal solution will also be assessed.

To complete the work on pin-wise power reconstruction, there are three ways to improve the prediction accuracy, those being to improve the prediction accuracy of the intra-nodal flux shape, improve the prediction accuracy of the intra-nodal kappa-sigma-
fission shape, and to introduce group power form factors. However, since the intra-nodal flux and kappa-sigma-fission both are predicted using results obtained from the nodal solution, the prediction accuracy of the nodal solution for mixed LEU-MOX cores enters.

This study is completed by using HELIOS, a transport theory based lattice physics code, and NESTLE, a diffusion theory core simulator. The single assembly (SA) calculation is done by HELIOS to generate the homogenized cross sections, discontinuity factors (DFs) at corner points and surfaces, and power form factors using infinite-medium spectra. Homogenized cross sections and surface average DFs are generally used in diffusion calculations. Obviously, they are not that accurate because the effect from neighbors is ignored in SA calculations, hence introduce errors in diffusion calculations. The colorset (CS) calculation done by HELIOS is to generate the same information but now accounting for LEU-MOX interface effects, where a colorset denotes an LEU-MOX assembly infinite checkerboard loading. The intra-nodal flux distribution is obtained by a SA NESTLE calculation using the finite difference method with a very fine spatial mesh. The surface current boundary condition imposed is obtained from the CS HELIOS calculation, with the NESTLE calculation completed using SA HELIOS determined homogenized cross sections or CS HELIOS determined intra-nodal cross sections.

The shape of intra-nodal cross section shows that the thermal group “flat” cross section can not represent the interfacial effect. This assumption no longer works for mixed LEU-MOX cores. The group dependent “flat” cross sections contribute errors to the $k_{eff}$, intra-nodal fluxes and powers.
Comparing the cross sections, DFs, and power form factors from SA lattice physics, CS lattice physics, and diffusion theory calculations, we can evaluate the errors induced by the MOX and LEU spectrum interactions on these values. Contrasting SA lattice physics and diffusion theory (using intra-nodal cross sections) predictions, for the SA lattice physics predictions about a 1.5% relative error in the LEU fuel assembly and 2.2% relative error in the MOX fuel assembly are observed in the thermal group surface averaged DFs. The relative errors in the fast group ADF ratios are small. However about a 2.7% relative error is observed in the thermal group ADFs’ ratios at BOL. Likewise, about a 3% relative error in the LEU fuel assembly and 4.4% relative error in the MOX fuel assembly are observed in the thermal group corner point DFs at BOL. Also about a 1% relative error is observed in $k_{\infty}$ in both the LEU and MOX fuel assemblies at a higher level burnup (20 GWD/THM). With regard to the intra-nodal cross sections, stronger spatial dependences are noted for the down-scattering, thermal transport, fast and thermal absorption, and fast and thermal fission cross sections. A steep spatial gradient is noted for the intra-nodal flux due to interfacial effects. The resulting flux shape presents a difficulty problem to accurately functionalize.

The study on the effect of ADF’s and cross sections shows that errors in the cross sections, i.e. the energy and spatial spectrum used for generating the cross sections, are the main error contributors to the $k_{\text{eff}}$, node averaged fluxes and intra-nodal fluxes. ADFs do not greatly effect the $k_{\text{eff}}$ value and node averaged fluxes.

The results of the study imply that the accuracy of the SA lattice physics calculation to obtain cross sections, DFs and form factors are poor for the mixed LEU-
MOX core simulations, in other words, the rehomogenization of cross sections is necessary during the nodal (diffusion theory) calculation for mixed LEU-MOX core simulations. Also, the employment of intra-nodal cross section is effective in improving the accuracy of diffusion calculation.
Intra-nodal Study for the Mixed LEU-MOX Cores

by

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1. Introduction

1.1. Background and Problem Description

People hope to take advantage of nuclear energy peacefully. There is a considerable quantity of weapon’s grade plutonium (WGPu), with about 94% fissile content, in the world. A surplus of WGPu exists in the United States and Russia due to drastic reductions in their nuclear weapon’s programs. One favored method being considered for the disposal of WGPu is to burn the WGPu as mixed oxide (MOX) fuel in commercial existing Light Water Reactors (LWRs). Duke Power Company intends to irradiate MOX fuel assemblies in their four Westinghouse pressurized water reactors (PWR) in support of reducing the United States stockpile. This implies that it is necessary to determine near-optimum fuel loading patterns satisfying reactor design constraints for mixed LEU-MOX cores by some core simulator. However, the introduction of MOX fuel into LWRs poses several challenges for the reactor physics analysis incorporated in core simulators.

What makes the mixed LEU-MOX core problem so different from the normal low enrichment uranium (LEU) core problem? It is because of the blackness relative to thermal neutrons of MOX fuel, which induces a steep spatial gradient in the thermal flux at the interface between the LEU and MOX fuel assemblies and makes the energy spectrum in the mixed LEU-MOX core a strong function of spatial position. We know that Pu-239, the main component of Pu in the MOX fuel, has a strong absorption ability to thermal neutrons. The microscopic thermal group absorption cross section of Pu-239 is 1221 barns. By contrast the microscopic thermal group absorption cross section of uranium-235 is just 282 barns.

The difference in properties of uranium and plutonium induces energy spectrum differences between the MOX and LEU assemblies, i.e., the energy spectrum in the MOX fuel assembly is much harder than that in the LEU fuel assembly, which creates a large thermal flux spatial gradient at the interface between these assemblies. The current methods for predicting the intra-nodal flux distribution have difficulty to model this gradient. Particularly, the methods employed in FORMOSA-P, which Duke Power Company is going to utilize for fuel management calculations, have large errors in predicting the corner point fluxes and pin wise fluxes for the mixed LEU-MOX core.

Generally, core simulator calculation using a nodal method consists of the steps of solving the diffusion equation over the reactor core using homogenized (including intra-nodal) cross sections and DFs, and then doing the pin-wise reconstruction utilizing the results of the homogenization and core-wide solution steps employing a number of assumptions. The basis
of the first step is to preserve the node-averaged reaction rates and surface currents as predicted by transport theory in the few-group, coarse mesh, diffusion theory calculation. This is accomplished by defining homogenized cross sections based upon flux-volume weighting and introducing surface average discontinuity factors (DFs).

The homogenized cross sections, DFs, and form factors are obtained from a single assembly (SA) calculation completed by a lattice physics code, such as CASMO, HELIOS, etc., for a single-lattice with a zero current boundary condition, \( i.e. \) infinite repetitive lattice in the radial plane. This introduces errors in both the lattice’s flux spatial distribution and isotopic spatial distributions resulting from depletion, since in practice the lattice in the core will be coupled to adjacent lattices via neutron transport. The SA calculation implies that these quantities are generated with totally different spectra from the real spectra. These quantities are the basic input for the diffusion calculation. In turn, this introduces errors into the results of diffusion calculation and pin-wise reconstruction, particularly, when the adjacent lattices have large neutronic property differences. How large the errors are in the lattice physics code generated data and how these errors will propagate to errors in the core simulator predicted quantities are the focuses of this thesis.

1.2. Sources of Errors

In practice, homogenized cross sections and DFs are part of basic inputs to the core simulation calculation, which determines node average quantities which are subsequently imposed as constraints in pin-wise reconstruction. With the help of the form factors, the heterogeneous pin-wise powers can be obtained. From the above procedure, we can see how the errors in the cross sections, DFs and form factors pass to the pin-wise power distribution.

The pin-power reconstruction is a very important part of reactor physics calculations. The knowledge of the detailed pin-power values are required in many reactor safety analysis. Current methods do a good job in predicting the pin-wise power for pure LEU or MOX cores, but they performed badly for mixed LEU-MOX cores.

The possible sources of errors can be divided into two catalogs. Firstly, the errors are brought in by the basic cross sections from the single assembly calculation. The two group cross sections used in the nodal method are usually obtained from infinite-lattice calculations for each type of fuel assembly with total reflection, \( i.e. \) zero current, boundary condition. These calculations do not take into account the large thermal flux gradient at the interface between the MOX and LEU. Further, two group cross sections from single assembly calculations are collapsed using the infinite medium energy spectra. In other words, the cross
sections of MOX fuel assembly are collapsed with the infinite MOX spectrum and those of LEU fuel assembly are collapsed with the infinite LEU spectrum. In the actual mixed LEU-MOX cores, the spectrum is neither ‘pure’ LEU nor MOX. Furthermore, the energy spectrum in the mixed LEU-MOX cores is strongly spatial dependent. The employment of a spatially ‘flat’ cross section within a node is no longer an acceptable assumption. Therefore, the two group cross sections from single assembly calculations may be a major source of the errors.

Secondly, pin-power errors are introduced by the assumptions we make for the spatial functional forms of some quantities.

1) Nodal solution quantities: surface average homogeneous flux, node average flux and surface average current. The current reactor physics computational methodology is based on the nodal expansion methods (NEM) [17] for solving the 3-D diffusion equation. Most nodal methods use the transverse integration procedure to solve the multi-dimensional diffusion equations. This means that the multi-dimensional diffusion equations are integrated over the directions transverse to each direction, therefore the multi-dimensional equations are reduced to a set of coupled one-dimensional equations. Generally, low order polynomials will be employed to approximate the transverse integrated fluxes. The transverse leakage in each direction, which provides the spatial coupling, is usually assumed to be a quadratic polynomial. Nodal solution quantities are obtained under these assumptions and with ‘flat’ cross sections within each node from the single assembly calculation. These assumptions and cross sections together contribute errors to these quantities. The errors in these quantities will be passed to the pin-wise reconstruction since we perform this reconstruction by preserving these quantities.

2) Corner point flux: We need more information than provided by the nodal solution to be part of the constraints used in determining the spatial distribution of the intra-nodal flux. To accomplish this, we introduce corner point fluxes as additional constraints, approximated by lower order polynomials. The method of obtaining the corner point flux together with corner point DFs will contribute additional errors on top of the nodal solution errors to the corner point flux.

3) Intra-nodal flux: How to obtain the intra-nodal flux accurately is very important to pin-wise reconstruction. Without special indication, the intra-nodal flux refers to the homogeneous intra-nodal flux, which should be spatially smooth to enable it to be modeled. As we discussed in section 1 of this chapter, there is a steep thermal flux gradient at the interface between the MOX and LEU fuel assemblies. Therefore, we have to choose the functional form for the intra-nodal flux carefully. For example, quartic polynomials are inadequate for the functional form of the thermal intra-nodal flux. In order to determine the
intra-nodal flux, nodal solution quantities and corner point fluxes are used as constraints. Obviously, errors will accumulate through the assumptions.

4) Intra-nodal kappa-sigma-fission: Generally lower order polynomials are employed to approximate this cross section by preserving the node average and surface average kappa-sigma-fission. This functional form may be inadequate because of the strong spatial and spectral dependence in the mixed LEU-MOX cores.

5) Pin-wise powers: Pin-wise powers are the final quantities we desire to determine. Usually, the homogeneous pin-wise powers are a product of the intra-nodal flux and intra-nodal kappa-sigma-fission. Then the heterogeneous pin-wise powers are obtained by multiplying the power form factor from the single assembly calculation with the homogeneous pin-wise powers. Obviously, contributors to the errors are the intra-nodal flux, intra-nodal kappa-sigma-fission and the power form factor.

We know the errors in the cross sections and computational models (e.g. functional form assumption, numerical methods) always exist in reactor physics calculations. It is impossible to eliminate these errors. However, lots’ of work has been performed and the results show that it is possible to model efficiently and accurately pure LEU or MOX reactor cores with acceptable errors. However, the mixed LEU-MOX cores present certain challenges for reactor physics computational methods. None the less, recent results in developing advanced methodologies have claimed that it is possible to model efficiently the effects of spectral interactions at interfaces between LEU and MOX assemblies [2].

1.3. Homogenization and Dehomogenization in Reconstruction

1.3.1 Homogenization

The lattice physics calculation is an important auxiliary calculation for the core simulation. For the assembly homogenization, two methods, the single assembly method and colorset method, can be used to perform the lattice physics calculations. In practice, to reduce computer time requirements, nearly always only the single assembly method is employed. The essential calculations of these methods are similar to each other. They solve a many group, two dimensional multigroup transport problem over the specified spatial domain with reflective boundary conditions on the outer edges of the domain. The results of the calculations are used to define average homogeneous few group cross sections for the assembly, as well as DFs and form factors. The difference between the two methods is that the single assembly calculation is performed over a symmetric quarter of a fuel assembly and the
reflective boundary condition is imposed on outer edges. By contrast, the colorset calculation is performed over four quarter assemblies which are adjacent to each other, and the reflective boundary condition is imposed on the centerlines of the fuel assemblies.

There is no doubt that inaccuracy may arise in SA calculations when the energy and spatial spectra in the real reactors are different from the spectra in the SA calculations. This is quite true for the mixed LEU-MOX cores due to the steep thermal flux gradient at the interface between the LEU and MOX fuel assemblies. The color set (CS) calculations automatically account for this gradient. This introduces intra-nodal effects that are reflected in the homogenization and dehomogenization processes. Obviously, it is more accurate than SA calculation. However, there are thousands upon thousands of possible color sets that must be run for each unique set of four-assembly configuration, particularly when used in support of determining the loading pattern as occurs in FORMOSA-P. Obviously, it is impractical for most reactor core calculations, especially when considering several fuel loading patterns involving assembly shuffling as done in incore fuel management studies. So in practice, what has been done is to utilize single assembly calculations and introduce some heterogeneity into the diffusion solution via the utilization of intra-nodal cross sections. These smoothly varying cross sections with spatial position within the node account in an approximate manner for intra-nodal effects.

The problem of how to correct the cross section from the SA calculation for intra-nodal effects must be addressed if this approach is utilized. Recently a method for leakage and spectral corrections of cross sections obtained in single assembly calculations was developed and became part of the SIMULATE methodology [2], [3]. This approach claims to reduce the error introduced by the single assembly calculations. Under separate work, this approach is being implemented in FORMOSA-P along with the transverse integrated nodal flux expanded in hyperbolic functions, which are more able to capture the spatial shape of the flux. In this thesis, it will be shown later how large the differences are in the homogeneous cross section generated by the single assembly calculations and colorset calculation for the mixed LEU-MOX. This is of relevance to the separate work just noted.

1.3.2 Reconstruction

Besides the nodal average flux, and surface average flux and current, advanced nodal methods provide limited information regarding the intra-nodal flux distribution [3]-[8], [11], [13], [14]. In fact, in most advanced models, the available intra-nodal flux distribution is limited to the one dimensional flux shape in each direction. This limitation is because of the
commonly employed transverse integration procedure. The assumption of flux separability in each direction does a poor job in predicting the actual 2-D intra-nodal flux distribution. This spatial information is necessary to estimate the pin-wise power distribution, in particular peak pin power values.

Several methods have been developed within the last two decades to estimate the intra-nodal flux. The first successful method of obtaining accurate intra-nodal flux distributions was introduced by Koebke et al.[6] and by Koebke and Wagner [7] by assuming that the intra-nodal flux distribution could be approximated by non-separable polynomials. However, the low order polynomials they employed can not accurately model the large localized gradients occurring at the assembly interfaces. This is especially true for mixed LEU-MOX cores. Another successful method was developed by K. S. Smith [9]-[11]. In this method, a high order non-separable polynomial is used for the fast intra-nodal flux shape, and a non-separable polynomial combined with hyperbolic sin and cosine functions is used for the thermal intra-nodal flux shape. Note that this method was employed in FORMOSA-P, and has been shown to predict the intra-nodal flux shape accurately for pure LEU or MOX cores. Unfortunately, it also has been shown to do a poor job for the mixed LEU-MOX core.

Recently, the challenges posed by the mixed LEU-MOX cores have prompted the development of improved methods. S. Palmtag proposed to modify the form of the 2-D intra-nodal homogeneous flux shape and obtain it, including the flux at the corners of each node, as part of the nodal solution [3], [12] versus post-processed as was the practice. This modified method approximates fluxes with a two-dimensional, non-separable functional form in terms of a combination of polynomial and hyperbolic sin and cosine function. The intra-nodal flux calculations are embedded in the nodal expansion method. Therefore, the post-processing to obtain the 2-D intra-nodal flux required in pin-wise reconstruction is not needed any more.

Because of the use of spatially homogenized cross sections in most nodal models, only the smooth intra-nodal flux distribution within each node can be obtained. In other words, the detailed pin-by-pin flux and power distributions are not immediately available from a nodal solution. However, the knowledge of detailed pin-wise information is required by the reactor safety analysis. Definitely, the fluxes within water holes, burnable absorbers, and fuel pins are significantly different from each other. Form factors are needed to recover the pin-wise introduced heterogeneities. There are two types of form factors commonly used: the group-wise power form factor [5] and the one-group power form factor [11], [13]. If the fast group contribution to the pin-wise power is relatively smooth, it is possible to use the one-group power form factor. This is true for the pure LEU or MOX cores. The group-wise form factor method has been shown to predict the pin-wise powers marginally better in a mixed LEU-
MOX core [4], [14].

Most reactor core simulators have the capability of pin-wise reconstruction. As noted above, the heterogeneous pin-wise powers are reconstructed using the homogeneous results from the nodal calculation, and form factors from lattice physics calculations. To impose the continuity of the actual heterogeneous fluxes, rather than the homogeneous nodal fluxes, at the surfaces, DFs are imbedded in the nodal codes so as to attempt to preserve node surface average currents. DFs for the corner points are also used in reconstruction methods. The DFs of an assembly are assumed to be insensitive to its neighbors. The result from the calculation for the DFs, discussed in a later section, shows that this assumption may not stand for the mixed LEU-MOX cores. This implies that the reference homogeneous surface averaged fluxes and corner point fluxes obtained by dividing the heterogeneous values from the colorset lattice calculation by the related DFs have errors. No published paper has mentioned how to correct the DFs for the mixed LEU-MOX cores.

As noted earlier, additional constraints other than the nodal solution quantities are required in predicting the intra-nodal flux distributions. These additional constraints involve fluxes, and sometimes currents, at the corner points of the node. How accurate the corner point fluxes are will strongly effect the prediction accuracy of nearby pin fluxes. Several methods compared in this work have shown that the errors in the nearby pin fluxes prediction are unacceptable.

To improve the prediction accuracy of reconstruction, three approaches can be taken: (i) improve the prediction accuracy of the intra-nodal flux shape, (ii) improve the prediction accuracy of the intra-nodal kappa-sigma-fission shape, and (iii) introduce group-wise power form factors. Some earlier work at NC State had be done about trying different functional forms for the intra-nodal flux shape, and using group-wise form factors based on homogenized cross sections. However, the solution accuracy was determined to be quite bad by comparing with reference values obtained by solving CS calculations.

To provide guidance and verify the accuracy of pin-wise power predictions, color set lattice physics calculations were utilized. They directly provide benchmarks for the pin-wise powers and burnups. In addition, using color set and single assembly lattice physics calculations, the following can be determined: 2-D (x, y) intra-nodal fluxes, powers, cross sections and burnups; 1-D transverse integrated cross sections and fluxes; and corner point fluxes and burnups. To verify the accuracy of the DFs and FFs from single assembly calculation, homogeneous finite difference calculations were performed using NESTLE [16]. The detailed procedure will be discussed later.
1.4. Scope of Research

Considerable work has been done on designing mixed LEU-MOX cores in some countries. This work is based on commercial grade plutonium (CGPu), which has about 67% fissile content blended down by natural or enrichment process tails uranium to a fairly low fissile content to produce the MOX fuel. However, WGPu has a much higher fissile content. WGPu work has only been undertaken within the past several years. Past work is useful in defining what design and methods challenges need consideration for WGPu. Results of these studies provide the starting points of our research.

The objectives of this research project are to study how much the mixed LEU-MOX spectra affect the cross sections, DFs and form factors, and later affect the pin-wise flux and power distributions.

In the current version of FORMOSA-P, pin power reconstruction is completed by using a power form factor approach, with kappa-sigma-fission values fitted to a low order polynomial in (x, y) to account for intra-nodal burnup and spectral history effects. Studies have been completed in regard to the accuracy of FORMOSA-P for a mixed LEU-MOX core application [4] by contrasting predictions using FORMOSA-P with color-set HELIOS predictions. FORMOSA-P and HELIOS predictions for key core attributes agreed well for the pure LEU and MOX color-sets, but poor for the mixed LEU-MOX color-set. To date, no work has been completed on analyzing the sources of the errors and how much these sources contribute to the errors in other quantities. Hence, the goal of this aspect of the study is to analyze the errors in the cross sections, DFs, form factors, intra-nodal flux, kappa-sigma-fission, and powers. Specifically, this study will address the following:

1. Compare the homogenized cross sections obtained from single assembly and color set calculations.
2. Compare surface cross sections at surface burnup level predicted by interpolation using the information from single assembly and color set calculations.
3. Calculate the relative intra-nodal cross section shape to check whether the ‘flat’ cross section assumption is acceptable or not.
4. Study the relative difference between the intra-nodal fluxes obtained from the diffusion calculation (NESTLE) and that from the transport calculation.
5. Compare the reaction rates obtained from color set and diffusion calculations.
6. Study the relative difference in the group-wise form factors obtained from SA calculation and CS combining diffusion calculations.
7. Evaluate the relative shape of intra-nodal fluxes.
8. Evaluate the DFs using the information from color set and diffusion calculations. Items 1 and 2 show errors due to ignoring interfacial effects. Item 3 shows the shapes of the intra-nodal cross sections. Item 4 shows the difference in the intra-nodal flux obtained from the diffusion equation and transport equation. Item 5 shows errors in reaction rates due to using diffusion equation. Item 6 shows the error in group dependent power form factor due to ignoring interfacial effects. Item 7 shows the shape of the intra-nodal flux. Item 8 shows the error in the DFs due to ignoring the interfacial effects.

The work covered in this study includes generation of reference data obtained from the HELIOS [15] lattice physics calculation, solving the diffusion equation using NESTLE to get the homogenized solution, coding the buffer codes to read the lattice physics code’s outputs to create the cross section inputs for NESTLE, and error analysis by comparing different approaches. Note that both LEU and MOX fuel assembly configurations utilized in this study are limited to the existing Westinghouse 17x17 style fuel assembly configuration.

1.5. Thesis Organization

Chapter 2 presents the basic methodology of the study adopted. Chapter 3 presents the errors in homogenized cross sections due to ignoring the interfacial effects and the spatial shape of the intra-nodal cross sections. Since they play an important role in diffusion calculations, a detailed discuss is addressed in this chapter. Chapter 4 is devoted to discussing the intra-nodal flux distribution and difference in the intra-nodal flux as obtained from the diffusion equation and transport equation. Chapter 5 presents the errors in the DFs, form factors, and reaction rates. Chapter 6 presents conclusions regarding this work and recommendations for future work.
2. Methodology

2.1. Methods in Dehomogenization Process

2.1.1 Pin-Wise Power Reconstruction Method

The wildly employed pin-wise power reconstruction method of Smith [11] is employed in FORMOSA-P. The idea of this method is that the heterogeneous pin-wise power distribution model is based on the one-group power form factor as follows:

\[ P^{(p)} = (P^{(p)})^{\text{Intra}} (FF^{(p)}) , \]

where

\[ (P^{(p)})^{\text{Intra}} = \sum_{g=1}^{2} (\kappa\Sigma_{fg}^{(p)})^{\text{Intra}} (\phi_{g}^{(p)})^{\text{Intra}} , \]

and \( (P^{(p)})^{\text{Intra}} \) denotes the intra-nodal pin powers, and \( (\kappa\Sigma_{fg})^{\text{Intra}} \) and \( (\phi_{g})^{\text{Intra}} \) denote the two-group intra-nodal kappa-sigma-fission cross section and flux, respectively, for pin “p”. \( FF^{(p)} \) denotes the one-group power form factor derived from SA lattice physics calculations:

\[ FF^{(p)} = \frac{\sum_{g=1}^{2} (\kappa\Sigma_{fg}^{(p)})^{\text{SA}} (\phi_{g}^{(p)})^{\text{SA}}}{\sum_{g=1}^{2} \langle \kappa\Sigma_{fg} \rangle^{\text{SA}} \langle \phi_{g} \rangle^{\text{SA}}}, \]

where \( (\kappa\Sigma_{fg}^{(p)})^{\text{SA}} \) and \( (\phi_{g}^{(p)})^{\text{SA}} \) denote the two-group pin-wise kappa-sigma-fission cross section and flux, respectively, and \( \langle \kappa\Sigma_{fg} \rangle^{\text{SA}} \) and \( \langle \phi_{g} \rangle^{\text{SA}} \) denote the homogenized node averaged kappa-sigma-fission cross section and flux, respectively. Obviously, the accuracy of the pin power predictions depends on the accuracy of the intra-nodal flux and cross section values in Eq. (2-2), and the form factors.

The current pin reconstruction method in FORMOSA-P works well for a pure LEU or MOX core, but poor for a mixed LEU-MOX core [4]. Hence, we introduce a two-group form factor functionalization in the pin-wise power prediction. We expect it to be more accurate in predicting the pin-wise powers. The two-group formulation is given by:
\[ P^{(p)} = \sum_{g=1}^{2} \left( P_{g}^{(p)} \right)^{\text{Intra}} \left( FF_{g}^{(p)} \right), \]  

(2-4)

where

\[ \left( P_{g}^{(p)} \right)^{\text{Intra}} = \left( \kappa \Sigma_{fg}^{(p)} \right)^{\text{Intra}} \left( \phi_{g}^{(p)} \right)^{\text{Intra}}, \]  

(2-5)

\[ FF_{g}^{(p)} = \frac{\left( \kappa \Sigma_{fg}^{(p)} \right)^{\text{SA}} \left( \phi_{g}^{(p)} \right)^{\text{SA}}}{\left( \kappa \Sigma_{fg}^{\text{SA}} \right) \left( \phi_{g}^{\text{SA}} \right)}. \]  

(2-6)

From [4], it was shown that the two-group form factor approach modestly improves the overall accuracy of the pin power distributions for all types of cores.

### 2.1.2 Corner Point Flux Approximation

Corner point flux values are currently used to act as constraints in determining the intra-nodal flux. Hence, the accuracy of corner point flux estimates will impact the accuracy of the pin-wise power prediction. The information from the nodal solution employing the transverse integrated nodal method, that being surface averaged and node volume averaged values of flux and/or current, do not contain sufficient information to directly determine the corner point fluxes. There are many approximate methods to predict the corner point fluxes.

**A. Smith’s Method.**

The original approach used in FORMOSA-P to determine the corner point flux adopted Smith’s method [11], which is based on the assumption that the flux can be separated into the x and y directions. Making this assumption, the homogeneous corner point flux is approximately determined by:

\[ \left( \phi_{g}^{\text{NW.hom}} \right)_{i} = \frac{\left( \bar{\phi}_{g}^{x}(-0.5) \right)_{i} \left( \bar{\phi}_{g}^{y}(0.5) \right)_{i}}{\left( \phi_{g} \right)_{i}}, \]  

(2-7)

where \( \left( \bar{\phi}_{g}^{x}(-0.5) \right)_{i} \) and \( \left( \bar{\phi}_{g}^{y}(0.5) \right)_{i} \) are the two-group transverse-integrated flux in the x and y directions, respectively, for node i evaluated at the surfaces, and \( \left( \phi_{g} \right)_{i} \) is the node averaged flux. The heterogeneous corner point flux is then obtained by averaging four adjacent nodes’ heterogeneous corner pointer flux values:
where the CPADF are the two-group corner point assembly discontinuity factors from single assembly lattice physics calculations. The rational for this approach is that the heterogeneous flux is continuous in space everywhere. This method is the most economical method with respect to computational cost.

Unfortunately, previous studies [4] showed that this method does not work well in a mixed LEU-MOX core environment where strong thermal flux gradients exist, especially at the corner points of the LEU-MOX interfaces. The same result was obtained during this work.

B. Koebke and Hetzelt’s Method.

An alternate method is the method of Koebke and Hetzelt [5]. It involves a four-node (see Figure 2-1) coupled problem with 32 unknowns to solve for. The functional form for this approach for node i is given as follows:

\[
\begin{align*}
(\phi_i)_{g,\text{Intra}} &= (a_{g0} + a_{g1}x + a_{g2}y + a_{g3}xy + a_{g4}x^2 + a_{g5}y^2 + a_{g6}xy^2 + a_{g7}x^2y)_i, \\
&= \frac{1}{4}((\text{CPADF}^{\text{NE}}_{g} \phi_{g,\text{NE,hom}} + \text{CPADF}^{\text{SE}}_{g} \phi_{g,\text{SE,hom}} + \text{CPADF}^{\text{SW}}_{g} \phi_{g,\text{SW,hom}} + \text{CPADF}^{\text{NW}}_{g} \phi_{g,\text{NW,hom}})_{1} + (\text{CPADF}^{\text{NE}}_{g} \phi_{g,\text{NE,hom}} + \text{CPADF}^{\text{SE}}_{g} \phi_{g,\text{SE,hom}} + \text{CPADF}^{\text{SW}}_{g} \phi_{g,\text{SW,hom}} + \text{CPADF}^{\text{NW}}_{g} \phi_{g,\text{NW,hom}})_{2} + (\text{CPADF}^{\text{NE}}_{g} \phi_{g,\text{NE,hom}} + \text{CPADF}^{\text{SE}}_{g} \phi_{g,\text{SE,hom}} + \text{CPADF}^{\text{SW}}_{g} \phi_{g,\text{SW,hom}} + \text{CPADF}^{\text{NW}}_{g} \phi_{g,\text{NW,hom}})_{3} + \text{CPADF}^{\text{NE}}_{g} \phi_{g,\text{NE,hom}} + \text{CPADF}^{\text{SE}}_{g} \phi_{g,\text{SE,hom}} + \text{CPADF}^{\text{SW}}_{g} \phi_{g,\text{SW,hom}} + \text{CPADF}^{\text{NW}}_{g} \phi_{g,\text{NW,hom}})_{4}),
\end{align*}
\]  

Figure 2-1. Node Configuration for Corner Point Flux Calculations.

where the CPADF are the two-group corner point assembly discontinuity factors from single assembly lattice physics calculations. The rational for this approach is that the heterogeneous flux is continuous in space everywhere. This method is the most economical method with respect to computational cost.

Unfortunately, previous studies [4] showed that this method does not work well in a mixed LEU-MOX core environment where strong thermal flux gradients exist, especially at the corner points of the LEU-MOX interfaces. The same result was obtained during this work.

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\[
(\phi_i)_{g,\text{Intra}} = (a_{g0} + a_{g1}x + a_{g2}y + a_{g3}xy + a_{g4}x^2 + a_{g5}y^2 + a_{g6}xy^2 + a_{g7}x^2y)_i, \\
= \frac{1}{4}((\text{CPADF}^{\text{NE}}_{g} \phi_{g,\text{NE,hom}} + \text{CPADF}^{\text{SE}}_{g} \phi_{g,\text{SE,hom}} + \text{CPADF}^{\text{SW}}_{g} \phi_{g,\text{SW,hom}} + \text{CPADF}^{\text{NW}}_{g} \phi_{g,\text{NW,hom}})_{1} + (\text{CPADF}^{\text{NE}}_{g} \phi_{g,\text{NE,hom}} + \text{CPADF}^{\text{SE}}_{g} \phi_{g,\text{SE,hom}} + \text{CPADF}^{\text{SW}}_{g} \phi_{g,\text{SW,hom}} + \text{CPADF}^{\text{NW}}_{g} \phi_{g,\text{NW,hom}})_{2} + (\text{CPADF}^{\text{NE}}_{g} \phi_{g,\text{NE,hom}} + \text{CPADF}^{\text{SE}}_{g} \phi_{g,\text{SE,hom}} + \text{CPADF}^{\text{SW}}_{g} \phi_{g,\text{SW,hom}} + \text{CPADF}^{\text{NW}}_{g} \phi_{g,\text{NW,hom}})_{3} + \text{CPADF}^{\text{NE}}_{g} \phi_{g,\text{NE,hom}} + \text{CPADF}^{\text{SE}}_{g} \phi_{g,\text{SE,hom}} + \text{CPADF}^{\text{SW}}_{g} \phi_{g,\text{SW,hom}} + \text{CPADF}^{\text{NW}}_{g} \phi_{g,\text{NW,hom}})_{4}),
\]  

There are 8 unknowns per node, so a total of 32 constraints are required, given by:

1. preserve node averaged flux, 1 constraint/node;
2. preserve surface averaged flux and current on interior surfaces, 4 constraints/node;
3. demand continuity of all corner point heterogeneous fluxes on interior surfaces, 7 constraints;
4. demand continuity of corner point currents on interior surfaces except the center, 4 constraints;
5. no net source at the center point, 1 constraint.
The coefficients of Eq. (2-9) can then be solved for, although the computation is expensive compared to some alternative methods denoted by Eq. (2-10). Setting \((x, y)\) to their values at the corner point in Eq. (2-9) produces the corner point flux value.

C. Polynomial Approximation.

One of the alternate methods which can be used to potentially improve the corner point flux calculation is the use of a 4th or 2nd-order polynomial functional form to approximate the intra-nodal flux within the node \(i\),

\[
(\phi_g)_i^{\text{Intra}} = (a_{g0} + a_{g1}x + a_{g2}x^2 + a_{g3}x^3 + a_{g4}x^4 + a_{g5}y + a_{g6}y^2 + a_{g7}y^3 + a_{g8}y^4)_i, \quad (2-10)
\]

or

\[
(\phi_g)_i^{\text{Intra}} = (a_{g0} + a_{g1}x + a_{g2}x^2 + a_{g3}y + a_{g4}y^2)_i, \quad (2-11)
\]

where \(x\) and \(y\) range from \(-1/2\) to \(1/2\). The corner point flux is obtained by substituting the \(x\) and \(y\) values that define the corner point. This intra-nodal functional form is only used to estimate the corner point fluxes. The unknown coefficients in Eq. (2-10) are determined by preserving the node and surface averaged flux and surface averaged current values. There are 5 unknowns in Eq. (2-11) and a total of 9 knowns from the nodal solution, which makes it necessary to select the constraints to impose. For example, we can pick the node and surface averaged flux values, or node averaged flux and adjacent surface flux and current values, as the constraints. The heterogeneous corner point flux can be then calculated by Eq. (2-8). From what had been observed [4], the polynomial method improves substantial the accuracy of the corner point flux prediction. Obviously, the computational cost of the polynomial approximations increases compared with Smith’s method, but decreases compared with Koebke and Hetzelt’s method.

D. Hybrid of Polynomial and Hyperbolic functional form.

In the mixed LEU-MOX core environment, the polynomial approximation may not be sufficient to evaluate the corner point fluxes at the interface of LEU and MOX fuel assemblies. Hence, the approximation of the hybrid of polynomial and hyperbolic functional form (see Eq. (2-12)) is tried during this study.

\[
(\phi_g)_i^{\text{Intra}} = (a_{g0} + a_{g1}x + a_{g2}x^2 + a_{g3}y + a_{g4}y^2)_i + a_{g5}\cosh(k_gx) + a_{g6}\sinh(k_gx) + a_{g7}\cosh(k_gy) + a_{g8}\sinh(k_gy))_i \quad (2-12)
\]
where \( k_g = \frac{\sum a_g \Delta x}{D_g} \) and \( x \) and \( y \) range from -1/2 to 1/2. Similar, the corner point flux is obtained by substituting the \( x \) and \( y \) values that define the corner point. The 8 unknowns in Eq. (2-12) are determined by preserving the node and surface averaged flux and surface averaged current values.

E. Polynomial Approximation with Cross-product Term.

The above methods are based on the assumption that the flux can be separated into the \( x \) and \( y \) directions. The actual flux is inseparable in each direction. The separation approximation will introduce an error into the corner point flux prediction. Hence, the following model was implemented in the code to study the accuracy of this model compared with the other methods. Figure 2-2 shows the node configuration for this method and the detailed expansion is shown in Eq. (2-13).

\[
(\phi_g)_{i}^{\text{Intra}} = (a_{g0} + a_{g1}x + a_{g2}
\left(3x^2 - \frac{1}{4}\right) + a_{g3}y + a_{g4}\n\left(3y^2 - \frac{1}{4}\right)) + a_{g5}xy + a_{g6}x\n\left(3y^2 - \frac{1}{4}\right) + a_{g7}\n\left(3x^2 - \frac{1}{4}\right)y)_i
\]  

(2-13)

where \( x \) and \( y \) range from -1 to 1. It is a 4-node coupled problem with 8 unknowns to solve for. The constraints adopted in this model are 4 node averaged flux values and 4 interior surface averaged flux values. Since the predicted corner point flux is shared by the 4 adjacent nodes, it is the heterogeneous flux we are fitting to. Due to the local coordinates, the corner point is always at (0,0) so the corner point flux is given as follows:

\[
(\phi_g)_i^{\text{Intra}} = \left(a_{g0} - \frac{a_{g2}}{4} - \frac{a_{g4}}{4}\right)_i
\]  

(2-14)
2.1.3 Intra-nodal Flux Approximation in Pin-Wise Power Reconstruction Method

A. Original Approach in FORMOSA-P.

We need to approximate the intra-nodal flux to complete pin-wise power reconstruction. The fast group intra-nodal flux shape currently used in FORMOSA-P is determined via a high order polynomial function:

\[
(\phi_1(x, y))^{\text{Intra}} = a_0 + \sum_{i=1}^{4} a_i x^i + \sum_{i=1}^{4} a_{i+4} y^i + \sum_{i=1}^{2} \sum_{j=1}^{2} a_{ij} x^i y^j. \tag{2-15}
\]

The 13 coefficients in Eq. (2-15) are determined by imposing as constraints the node averaged flux, 4 surface averaged fluxes, and 4 surface averaged currents all obtained from the nodal solution; and, 4 corner point fluxes that are estimated as noted above. The thermal group intra-nodal flux currently used in FORMOSA-P is composed of a particular solution due to the slowing down component, proportional to the fast group intra-nodal flux, and hyperbolic terms corresponding to the overtones associated with the analytic solution of a homogeneous node.

\[
(\phi_2(x, y))^{\text{Intra}} = b_0 \phi_1(x, y) + \sum_{i=1}^{2} \left( b_i \cosh(ik_x x) + b_{i+2} \sinh(ik_x x) \right) + \sum_{i=1}^{2} \left( b_{i+4} \cosh(ik_y y) + b_{i+6} \sinh(ik_y y) \right) + b_9 \cosh(k_x x) \cosh(k_y y) + b_{10} \cosh(k_x x) \sinh(k_y y) + b_{11} \sinh(k_x x) \cosh(k_y y) + b_{12} \sinh(k_x x) \sinh(k_y y) \tag{2-16}
\]

where \(k_x = \frac{\Sigma a_2}{\sqrt{D_2}} \Delta x\) and \(k_y = \frac{\Sigma a_2}{\sqrt{D_2}} \Delta y\), with \(\Sigma a_2\) and \(D_2\) denoting the thermal group absorption cross section and diffusion coefficient, respectively. Likewise, the 13 coefficients in Eq. (2-16) are determined by imposing constraints on the node, surface and corner point fluxes and/or currents as noted above.

B. Potential Approach with Consistency with Transverse Integrated Flux.

This method is not consistent with the transverse integrated fluxes obtained from the nodal solution. The following functional form for the intra-nodal flux:
where $\langle \Phi_g(x) \rangle$ and $\langle \Phi_g(y) \rangle$ are obtained from the nodal solution, does preserve the nodal solution. The unknown coefficients in Eq. (2-17) are determined by the corner point flux constraints. Whether preserving the 1-D fluxes obtained from the nodal solution is important is debatable since nodal methods only attempt to preserve surface averaged currents and node averaged flux, and do not explicitly address within-node flux spatial shape.

2.1.4 Intra-nodal Kappa-sigma-fission Approximations in Pin-Wise Power Reconstruction Method

A. Original Approach in FORMOSA-P.

Currently in FORMOSA-P, the intra-nodal kappa-sigma-fission spatial shape within a node is assumed to have a spatially separable low-order polynomial functional form:

$$ (\kappa \Sigma_{fg}(x, y))^{\text{Intra}} = a_0 + \sum_{i=1}^{2} a_i x_i + \sum_{i=1}^{2} a_{i+2} y_i. \quad (2-18) $$

The coefficients of Eq. (2-18) are determined by requiring the node volume and 4 surface averaged intra-nodal $\kappa \Sigma_{fg}$ values to be preserved. This low order polynomial approximation for kappa-sigma-fission in the mixed LEU-MOX cores may be inadequate.

B. Potential Approach with Consistency with 1-D Kappa-sigma-fission.

Since transverse integrated 1-D cross sections with spectral correction are being introduced into our nodal problem, we can demand consistence between the intra-nodal and transverse integrated 1-D fission cross section functionalizations, which Eq. (2-18) does not do. Similar to the intra-nodal flux functionalization, we can postulate a intra-nodal kappa-sigma-fission of the following form:

$$ (\kappa \Sigma_{fg}(x, y))^{\text{Intra}} = \frac{\langle \kappa \Sigma_{fg}(x) \rangle \langle \kappa \Sigma_{fg}(y) \rangle \langle \Phi_g(x) \rangle \langle \Phi_g(y) \rangle}{\langle \kappa \Sigma_{fg} \rangle \langle \Phi_g \rangle \langle \Phi_g(x, y) \rangle^{\text{Intra}}}. \quad (2-19) $$

This formulation makes the intra-nodal fission cross section consistent with the transverse integrated 1-D fission cross section in spatial shape and preserves the reaction rate. But this form is very complicated. However, no intra-nodal flux and kappa-sigma-fission calculations
are needed because we can calculate group intra-nodal powers by using only the transverse integrated and node averaged flux and kappa-sigma-fission cross section. The group averaged pin-wise intra-nodal power can be obtained by integrating the intra-nodal power shape over each pin cell and dividing the volume of the pin cell. This approach is not expected to be accurate because just like flux, group power is not expected to be separable in x and y.

C. High Order Polynomial Approximation.

An alternate higher order polynomial functional form than currently used can be implemented:

\[
(\kappa \Sigma_{fg} (x, y))^{\text{Intra}} = a_0 + \sum_{i=1}^{2} a_i x^i + \sum_{i=1}^{2} a_{i+2} y^i + \sum_{i=1}^{2} \sum_{j=1}^{2} a_{ij} x^i y^j .
\] (2-20)

The additional 4 coefficients can be determined by preserving corner point \(\kappa \Sigma_{fg}\) values. They can be estimated by interpolating with respect to burnup the kappa-sigma-fission to the burnup value at the corner.

2.2. True Intra-nodal Flux and Cross Sections

2.2.1 True Intra-nodal Flux

To address the inadequacies associated with SA calculations, four adjacent assemblies, \textit{i.e.} lattices, are analyzed by HELIOS via SA and CS calculations. The focus of the work is to determine whether the introduction of intra-nodal cross sections will be effective for mixed LEU-MOX cores, as is the case for pure LEU cores, and to determine appropriate intra-nodal cross sections. Once these determinations have been made, assuming positive results, then one can subsequently decide on how in a practical manner for routine core design calculations one can obtain the intra-nodal cross sections. We now present the definition of intra-nodal quantities.

The intra-nodal flux can be defined as the spatially smooth flux component that results when intra-nodal effects are treated. This implies that in terms of SA and CS lattice physics calculations,

\[
\Phi^{(CS)}_g (x, y) = f^\Phi_g (x, y) \Phi^{(Intra)}_g (x, y) ,
\] (2-21)

where the flux form factor is defined as
and the node-averaged SA flux as
\[ \langle \phi_g^{(SA)} \rangle = \frac{\int \int \phi_g^{(SA)}(x, y) dx dy}{\int \int dx dy}, \]  
(2-23)
with the span of the surface integration over a lattice. Eq. (2-21) and Eq. (2-22) can be used to solve for the intra-nodal flux,
\[ \phi_g^{(Intra)}(x, y) = \frac{\phi_g^{(CS)}(x, y)}{\langle \phi_g^{(SA)} \rangle} \langle \phi_g^{(SA)} \rangle. \]  
(2-24)
If integrated over either the \( x \) or \( y \) dimension in Eq. (2-24), one obtains the 1-D intra-nodal flux which we hope the transverse-integrated diffusion equation to render. We also wish to preserve the node-averaged flux, so the intra-nodal flux defined by Eq. (2-24) must be normalized as
\[ \tilde{\phi}_g^{(Intra)}(x, y) = c_g \phi_g^{(Intra)}(x, y), \]  
(2-25)
where
\[ c_g = \frac{\int \int \phi_g^{(CS)}(x, y) dx dy}{\int \int \phi_g^{(Intra)}(x, y) dx dy}, \]  
(2-26)
which assures that
\[ \int \int \phi_g^{(Intra)}(x, y) dx dy = \int \int \phi_g^{(CS)}(x, y) dx dy. \]  
(2-27)

### 2.2.2 True Intra-nodal Cross Sections

In a like fashion we can define the intra-nodal cross section as follows, which represents the smoothly varying portion of the cross section:
\[ \Sigma_{xg}^{(CS)}(x, y) = f_{xg}(x, y) \Sigma_{xg}^{(Intra)}(x, y), \]  
(2-28)
where the cross section form factor is defined as
\[ f_{xg}(x, y) = \frac{\Sigma_{xg}^{(SA)}(x, y)}{\langle \Sigma_{xg}^{(SA)} \rangle}, \]  
(2-29)
and the node-averaged SA cross section as
\[
\langle \Sigma_{xg}^{(SA)} \rangle = \int \int \Sigma_{xg}^{(SA)}(x, y) \phi_g^{(SA)}(x, y) dxdy / \int \int \phi_g^{(SA)}(x, y) dxdy.
\] (2-30)

Eq. (2-28) and Eq. (2-29) can be used to solve for the intra-nodal cross section,
\[
\Sigma_{xg}^{(Intra)}(x, y) = \frac{\Sigma_{xg}^{(CS)}(x, y)}{\Sigma_{xg}^{(SA)}(x, y)} \langle \Sigma_{xg}^{(SA)} \rangle.
\] (2-31)

As was the case with the intra-nodal flux, we desire the intra-nodal cross section to preserve the node-averaged reaction rate, which requires a normalization given by
\[
\Sigma_{xg}^{(Intra)}(x, y) = c_{xg} \Sigma_{xg}^{(Intra)}(x, y),
\] (2-32)

where
\[
c_{xg} = \int \int \Sigma_{xg}^{(CS)}(x, y) \phi_g^{(CS)}(x, y) dxdy / \int \int \Sigma_{xg}^{(Intra)}(x, y) \phi_g^{(Intra)}(x, y) dxdy.
\] (2-33)

which assures that
\[
\int \int \Sigma_{xg}^{(Intra)}(x, y) \phi_g^{(Intra)}(x, y) dxdy = \int \int \Sigma_{xg}^{(CS)}(x, y) \phi_g^{(CS)}(x, y) dxdy.
\] (2-34)

### 2.2.3 True Discontinuity Factors

The true DFs is defined as following:
\[
ADF_g = \langle \phi_g^{(Intra)} \rangle^{(S)} / \langle \phi_g^{(Intra)} \rangle,
\] (2-35)
\[
CPDF_g = \langle \phi_g^{(Intra)} \rangle^{(CP)} / \langle \phi_g^{(Intra)} \rangle,
\] (2-36)

where (S) denotes surface, (CP) corner point, ADF denotes the surface averaged discontinuity factor, and CPDF the corner point discontinuity factor.

### 2.3. Difficulties

Needless to say, to determine the intra-nodal flux and cross sections as defined above requires both CS and SA lattice calculations. With CS calculations not being practical for routine nuclear design calculations, this indicates the above equations’ purpose is restricted to defining the true intra-nodal flux and cross sections values.
Will $\phi_g^{\text{Intra}}(x, y)$ obtained as just noted equal $\phi_g^{\text{Intra}}(x, y)$, which is the solution of fine-mesh diffusion calculation? Likely not. In fact the above equations do not define the true intra-nodal flux values. This is because the intra-nodal flux that we are interested in is the flux that results from the diffusion calculation, which will differ from that defined in Eq. (2-25). We can obtain the true intra-nodal flux by solving the diffusion equation with a fine mesh approach on a single-lattice, imposing the current along the lattice’s surfaces, which is determined by the CS lattice calculation, as the boundary condition in place of the zero current boundary condition. In the diffusion calculation we should utilize the intra-nodal cross sections, with the exception being that the diffusion coefficient is assumed to be spatially independent, \textit{i.e.} constant. The NESTLE diffusion theory code has been modified to allow the CS determined current boundary condition to be utilized. As just noted, to complete the diffusion calculation we also need to know the intra-nodal cross sections. From this calculation we can also determine the true DFs, defined as the ratio of the diffusion theory determined surface averaged flux to lattice averaged flux, and contrast their values with the DFs obtained by the standard approach, \textit{i.e.} from SA lattice calculations utilizing the same definition. Any errors in DFs translates to errors in the nodes’ surface averaged currents and hence core’s $k_{\text{eff}}$, node-wise power distribution, and intra-nodal flux, which will impact the pin-wise reconstruction. Also, we can determine the true pin-wise flux or power form factors from the diffusion equation solution and again contrast their values with those obtained in the standard approach, \textit{i.e.} from the SA lattice calculations.

Examining Eq. (2-33) we note a dilemma in what has just been proposed. To determine the diffusion theory based intra-nodal flux requires us to first know the intra-nodal cross sections. However Eq. (2-33) indicates that the intra-nodal flux must be know to determine the reaction rate preserving normalization factor. To be consistent, this intra-nodal flux should be based upon the diffusion equation solution and not the CS lattice calculation. There appears to be no obvious way to address this dilemma of mutual dependence; therefore, the intra-nodal cross sections will be determined using CS and SA lattice calculations as defined above. To determine the magnitude of errors introduced by this approximation, we will contrast the lattice reaction rates as predicted by diffusion calculations and lattice calculations, specifically

$$\int \int \Sigma_{xg}^{\text{Intra}}(x, y)\phi_g^{\text{Intra-Diff}}(x, y)dx dy$$  \hspace{1cm} (2-37)$$

$$\text{versus}$$

$$\int \int \Sigma_{xg}^{\text{CS}}(x, y)\phi_g^{\text{CS}}(x, y)dx dy$$  \hspace{1cm} (2-38)$$
where the superscript $\text{Diff}$ has been added to denote the diffusion calculation determined intra-nodal flux. It is also of interest to complete diffusion calculations utilizing the CS determined node-averaged cross sections, which by definition are spatially constant within a node. These calculational results would help us evaluate the merits of utilizing intra-nodal cross sections.
3. True Intra-nodal Cross Section

3.1. Study Case Description

The study of true intra-nodal cross section can be completed using results from SA and CS lattice physics calculation. The lattice physics code that was employed in this study is HELIOS, which employs the Current Coupling Collision Probability (CCCP) method to solve the 2-D integral form of the neutron transport equation. The many-group cross section library is based on ENDF/B-VI. In this study, the 45-group cross section library was used to collapse to 2-group cross sections for both the SA and CS calculation.

The CS lattice physics calculation is based upon a heterogeneous lattice. However, the intra-nodal cross sections that we are interested in are the cross sections that smoothly varying within the lattice. We need to extract the exact “intra-nodal” information from CS and SA lattice calculations as we described in chapter 2.

Figure 3-1 shows the CS problem solved by HELIOS. By extracting from the solution as described above, we can obtain the node average cross section, fluxes, corner point fluxes, surface average fluxes and currents, current distribution along the surfaces, and pin-wise fluxes, powers and kappa-sigma-fission.

<table>
<thead>
<tr>
<th>4.22 w/o LEU</th>
<th>4.37 w/o MOX</th>
</tr>
</thead>
<tbody>
<tr>
<td>(SEG = 3)</td>
<td>(SEG = 4)</td>
</tr>
<tr>
<td>NOBP</td>
<td>NOBP</td>
</tr>
<tr>
<td>FEED</td>
<td>FEED</td>
</tr>
<tr>
<td>4.37 w/o MOX</td>
<td>4.22 w/o LEU</td>
</tr>
<tr>
<td>(SEG = 1)</td>
<td>(SEG = 2)</td>
</tr>
<tr>
<td>NOBP</td>
<td>NOBP</td>
</tr>
<tr>
<td>FEED</td>
<td>FEED</td>
</tr>
</tbody>
</table>

Figure 3-1. Checkerboard MOX/LEU.

There are two types of Westinghouse 17x17 fuel assemblies (F/A), LEU and MOX, respectively, within this checkerboard benchmark calculation. Hence, two related SA calculations were completed for these types of fuel assemblies. Both SA and CS calculation are based upon heterogeneous geometry.
The detailed layout of the LEU fuel assembly is shown in Figure 3-2 (only quarter fuel assembly is shown because of symmetry). The diameter of fuel pins is 0.375 inch. The enrichment of fuel pins within the LEU fuel assembly is uniform, i.e. all 4.22 w/o. A instrument tube is located in the center of the LEU fuel assembly and a totally 24 guide tubes distribute within the fuel assembly.

Legend:  
- **UO$_2$**  
- **Zr**  
- **H$_2$O**

**Figure 3-2. Layout of LEU Fuel Assembly.**
The MOX fuel assembly is assumed to be a lattice with 0.375 in. diameter fuel pins (see Figure 3-3). The lattice is modeled after the Mark B&W fuel type used in McGuire and Catawba.

There are three types of fuel pins with different enrichments: 12 low enrichment pins of 2.35 w/o, 76 medium enrichment pins of 3.67 w/o, and 176 high enrichment pins of 4.81 w/o. The
pin-wise enrichment heterogeneity in the MOX fuel assembly is used in order to avoid high power peak near the assembly edge. This produces an averaged fuel pellet enrichment of 4.37 w/o. Down blending is done using depleted UO2 (0.23% U-235). Other assembly structure is similar with that of the LEU fuel assembly.

### 3.2. Node Averaged Cross Sections

Large relative differences are observed in several types of node-averaged (homogenized) cross sections as determined by HELIOS SA calculations versus those determined by HELIOS CS calculations, particularly in the thermal group cross sections. Figure 3-4 and Figure 3-5 show the relative differences in the diffusion coefficients, down scattering, absorption and nu-fission cross section as a function of burnup for the LEU and MOX lattices, respectively. Figure 3-6 and Figure 3-7 show the relative differences in \( k_{\infty} \) with burnup for the LEU and MOX lattices, respectively, where \( k_{\infty} \) is evaluated as

\[
k_{\infty} = \frac{\nu \Sigma_{f1} \Sigma_{a2} + \nu \Sigma_{f2} \Sigma_{s12}}{(\Sigma_{a1} + \Sigma_{s12}) \Sigma_{a2}}, \tag{3-1}
\]

and

\[
\text{Rel. Diff.} = \frac{(\text{SA Sol.} - \text{CS Sol.})}{\text{CS Sol.}} \tag{3-2}
\]

The relative differences in the fast group cross sections are small except for the fast nu-fission cross section both in the LEU and MOX fuel assemblies. Note that about a 3% difference occurs for the fast nu-fission both in the LEU and MOX fuel assemblies. As thought, the differences in the thermal group cross section are larger: about 3% difference of the thermal absorption cross section in the LEU fuel assembly and 3.6% difference in the MOX fuel assembly, and about 4.3% difference in thermal nu-fission cross section in the LEU fuel assembly and 4.8% difference in the MOX fuel assembly. Surprisingly, even the thermal group diffusion coefficient shows appreciable differences, these interfacial induced changes believed ignored in currently employed methods. The largest differences of the thermal diffusion coefficient occur at the beginning of life (BOL): about 1.5% difference in the LEU fuel assembly and 5% difference in the MOX fuel assembly. These differences occur at BOL due to instantaneous interfacial effects which change both the spatial and energy distributions of the neutron flux, which impact the homogenized cross section values. With burnup, these instantaneous effects accumulate as history effects in the altered spatial distributions of isotopic number densities, so that both instantaneous and history effects impact the CS homogenized cross section values when burnup is present. Note that many times the
differences in SA and CS cross section values of the LEU and MOX lattices are of similar magnitude but of opposite sign.

Figure 3-4. Rel. Difference in Cross Sections in LEU F/A.
The $k_\infty$ indicates the collective relative difference in the other types of cross sections. The difference of $k_\infty$ in the LEU fuel assembly becomes more negative with burnup. It reaches -0.0117 at the highest burnup level. Oppositely, the difference of $k_\infty$ in the MOX fuel assembly becomes more positive with burnup. It reaches 0.0111 at the highest burnup level. Larger absolute difference can be observed at higher burnups, specially for the case where transient fission products, i.e. Xe and Sm, effects are included in the $k_\infty$ calculation.

Figure 3-5. Rel. Difference in Cross Sections in MOX F/A.
Figure 3-6. Rel. Difference in $k_\infty$ in LEU F/A.
3.3. Renormalization Factors for Intra-nodal Cross Sections

As mentioned in chapter 2, we need to renormalize the intra-nodal cross section to preserve the reaction rates. Figure 3-8 through Figure 3-11 show the renormalization factors for the transport, absorption, nu-fission and down scattering cross sections in the LEU and MOX F/A as a function of burnup.

One can observe that the normalization factor for the fast transport coefficient either in
the LEU or in the MOX fuel assembly only fluctuates a little with burnup, but that for the thermal transport coefficient it does change more with burnup. The thermal group values are furthest from unity at the BOL. It is conjectured that the normalization factors are closed to 1.0 when the pin-wise spatial variations of the CS flux are less severe, which is true for the fast flux at all burnups and the thermal flux with burnup.

![Figure 3-8. Normalization Factor of Transport Coefficient.](image-url)
The normalization factor for the absorption cross section in the LEU and MOX fuel assemblies varies with burnup, although the variation is very small for the fast group. Again, deviation from 1.0 is the largest at BOL in the thermal group.

![Figure 3-9. Normalization Factor of $\Sigma_a$.](image-url)
Similar behavior is noted for the nu-fission cross section.

Figure 3-10. Normalization Factor of $\nu\Sigma_f$. 
The down scattering cross section is noted to be close to 1.0 for both the LEU and MOX lattices at all burnups.

Figure 3-11. Normalization Factor of $\Sigma_{s12}$. 
3.3.2 Intra-nodal Cross Section Shape

The intra-nodal cross section relative shapes are presented in Figure 3-12 through Figure 3-25 at 0 (BOL), ~0.5, ~10 and ~20 GWD/THM for LEU and MOX lattices. The intra-nodal cross section values have been normalized by dividing through by the node-averaged cross section values to better display the intra-nodal cross sections spatial variation. For cross section types that involve the fission cross section, we can see from Eq. (2-24) that the intra-nodal cross section for a non-fission region, e.g. water hole, is undefined since a zero divide by zero operation is involved. To address this problem, it is assumed that the cross section in a non-fission region is the average of the four adjacent unit cells’ cross section values. For the same problem that occurs in the water gaps, it is assumed that the cross section within the water gap is linearly extrapolated from the two nearest unit cells in each direction. This treatment is reflected in the normalization factors to assure node averaged reaction rates are preserved.

The spatial distribution at BOL is totally due to instantaneous intra-nodal spectra effects since no fuel depletion has yet taken place. The spatial distributions at ~0.5, ~10, and ~20 GWD/THM are due to not only instantaneous intra-nodal spectral effects, but also the history (cumulative) impact on the spatial distributions of the nuclei isotopics due to intra-nodal effects. Note that for all cross section types, the intra-nodal cross section is fairly flat about the lattice’s center, i.e. (0,0) of the figures. This is expected since this region of the lattice is furthest removed from the interfaces, so should experience an asymptotic flux spectrum, i.e. SA lattice flux spectrum. Stronger spatial dependence is noted for the downscatter, thermal transport coefficient, fast and thermal absorption, and fast and thermal fission cross sections. It is interesting to note that the fast absorption and fission cross sections are included in this list of cross sections with stronger spatial dependence, since intuitively given the greater mean free path of fast neutrons one would not expect the intra-nodal effect to be significant. This is conjectured to be due to the strong dependency of epi-thermal resonance capture on the fast flux spectrum. With regard to stronger dependence on burnup, the same cross section types as identified for stronger spatial dependence are involved. Note these observations apply to both LEU and MOX lattices.
Figure 3-12. Relative Shape of Transport Coefficient at BOL.
Figure 3-13. Relative Shape of Transport Coefficient at BU=500 MWD/THM.
Figure 3-14. Relative Shape of Transport Coefficient at BU=10 GWD/THM.
Figure 3-15. Relative Shape of Transport Coefficient at BU=20 GWD/THM.
Figure 3-16. Relative Shape of $\Sigma_{s,12}$ at BU=0, 500 MWD/THM.
Figure 3-17. Relative Shape of $\Sigma_{s,12}$ at $BU=10, 20$ GWD/THM.
Figure 3-18. Relative Shape of $\Sigma_a$ at BOL.
Figure 3-19. Relative Shape of $\Sigma_a$ at BU=500 MWD/THM.
Figure 3-20. Relative Shape of $\Sigma_\alpha$ at BU=10000 MWD/THM.
Figure 3-21. Relative Shape of $\Sigma_\alpha$ at BU=20000 MWD/THM.
Figure 3-22. Relative Shape of $\nu \Sigma_f$ at BOL.
Figure 3-23. Relative Shape of $\nu \Sigma_f$ at BU=500 MWD/THM.
Figure 3-24. Relative Shape of $\nu \Sigma_f$ at BU=10000 MWD/THM.
Figure 3-26 and Figure 3-27 show the maps of intra-nodal $k_\infty$ in the LEU and MOX fuel assemblies at BOL, 0.5, 10, and 20 GWD/THM. These values are evaluated with the normalized intra-nodal cross sections. Note that $k_\infty$ is fairly flat at the center of the fuel assembly. Stronger spatial dependence can be observed at the interface between the LEU and MOX fuel assemblies. The spatial behavior results due to the intra-nodal cross section spatial behavior.
Figure 3-26. Map of $k_{\infty}$ in LEU at Four Burnup Levels.
Figure 3-27. Map of $k_{\infty}$ in MOX at Four Burnup Levels.
3.4. Surface Averaged Cross Sections

Generally, the surface averaged cross sections, used as constraints on obtaining approximations to the intra-nodal cross sections, are obtained by interpolating to the surface averaged burnup level using the node averaged cross section as a function of node average burnup information from the SA calculation. In this section, the values obtained using this traditional approach will be compared with the values obtained by averaging the surface intra-nodal cross sections as a function of CS determined surface burnup level. The surface burnup is evaluated by linearly extrapolating from nearby adjacent nodes. A cubic spline is employed to extrapolate the cross section to the surface burnup level.

Figure 3-28 through Figure 3-32 show the interior and exterior surface averaged cross sections of the LEU and MOX fuel assemblies obtained by the two approaches as a function of surface average burnup. Note that the value of the interior surface burnup in LEU is higher than that of exterior surface burnup. This situation is reversed in MOX. The differences in the diffusion coefficients decreases as burnup increases. The differences for most other types of cross sections increase as burnup increases. This is conjectured to occur since the energy spectra on the surfaces about the LEU-MOX interface is substantially different than the lattice average energy spectra, which impacts isotopic reaction rates and hence number densities via depletion effects. This suggests that spectral history corrections must be applied to obtain more accurate surface average intra-nodal cross section estimates, a practice commonly employed. The maximum relative difference is about 4.4% in the LEU fuel assembly and 4.82% in the MOX fuel assembly both in the thermal nu-sigma-f cross section.
Figure 3-28. Interior Surface Averaged XS and $k_{\infty}$ in LEU.
Figure 3-29. Exterior Surface Averaged XS and $k_\infty$ in LEU.
CHAPTER 3: TRUE INTRA-NODAL CROSS SECTION

Figure 3-30. Interior Surface Averaged XS and $k_\infty$ in MOX.
Figure 3-31. Exterior Surface Averaged XS and $k_{\infty}$ in MOX.
Figure 3-32. Rel. Err. in Surface Averaged XS.
4. True Intra-nodal Flux

4.1. Boundary Condition Description

The study of intra-nodal flux can be completed using results from SA and CS lattice physics calculations (HELIOS), and diffusion calculations completed by NESTLE. The SA, CS and true intra-nodal cross sections have been used in diffusion calculations. This was done to help us understand how cross sections impact the intra-nodal flux distribution. The surface current distribution from the CS lattice calculation is imposed in the diffusion calculation as the boundary condition.

Figure 4-1 and Figure 4-2 show the surface average incoming current values from the HELIOS CS calculation. We can observe that the fast surface averaged currents are not exactly diagonally symmetric although the problem is a diagonally symmetric problem. This may be due to the accuracy of the numerical method employed by HELIOS. Also note that the fast neutrons ‘flow’ from the MOX fuel assembly into the LEU fuel assembly, and the thermal neutrons ‘flow’ from the LEU fuel assembly into the MOX fuel assembly. This behavior is expected due to the blackness of the MOX fuel to thermal neutrons and the large fission cross section for the MOX fuel.
### Figure 4-1. Fast Current Values at BOL from HELIOS.

<table>
<thead>
<tr>
<th></th>
<th>LEU 7.79711E-04</th>
<th>-7.79711E-04</th>
<th>MOX 0</th>
<th>7.79608E-04</th>
<th>-7.79607E-04</th>
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</tbody>
</table>
Figure 4-2 through Figure 4-6 show the fast and thermal incoming current spatial distributions along the surface at the interface between the LEU and MOX fuel assemblies from HELIOS CS calculation. ‘South’ in the legend of those figures indicates the south surface of the southeast quarter fuel assembly (same as the northwest quadrant in the checkerboard). ‘Cell number’ along the south surface counts from west to east for fuel pins and water gap. ‘East’ indicates the east surface of the southeast quarter fuel assembly. ‘Cell number’ along the east surface counts from north to south. Strong spatial dependence occurs about the center of the checkerboard due to approaching the interfaces of all four assemblies. Due to symmetry, the current must be zero at the center of the checkerboard.

Figure 4-2. Thermal Current Values at BOL from HELIOS.
Figure 4-3. Fast Surface Current Distribution in LEU.
Figure 4-4. Thermal Surface Current Distribution in LEU.
CHAPTER 4: TRUE INTRA-NODAL FLUX

Figure 4-5. Fast Surface Current Distribution in MOX.
4.2. Intra-nodal Flux Shape

The intra-nodal flux that we are interested in is the solution from the diffusion equation. This follows since the core-wide problem is analyzed using the diffusion equation. The diffusion results are based upon fine-mesh (2x2 per unit pin cell) finite difference NESTLE simulations employing homogenized cross section from either SA or CS calculations, and normalized intra-nodal cross sections as defined previously, to determine the intra-nodal flux. In all cases, surface current boundary conditions are imposed based upon the CS lattice (transport) solution.

Figure 4-6. Thermal Surface Current Distribution in MOX.
The CS intra-nodal flux shapes calculated by NESTLE utilizing the fine-mesh finite different method with the intra-nodal cross sections are shown in Figure 4-7 through Figure 4-10. For orientation purposes, the far edges of the figures denote the LEU-MOX lattice interfaces. Steep thermal flux gradients can be observed at the edges of the node, i.e. the interface of the LEU and MOX lattices. The resulting flux shape presents a difficult problem to accurately functionalize. Note that the interfacial effect becomes less and less with burnup.

Figure 4-7. Flux Shape by NESTLE Using $\Sigma_{xg}^{(Intra)}(x, y)$ at BOL.
Figure 4-8. Flux Shape by NESTLE Using $\Sigma_{xg}^{(Intra)}(x, y)$ at Bu=0.5 GWD/THM.
Figure 4-9. Flux Shape by NESTLE Using $\Sigma_{xg}^{(Intra)}(x, y)$ at Bu=10 GWD/THM.
The relative difference in the CS intra-nodal flux calculated by NESTLE using the node averaged cross sections from the CS transport calculation with respect to the values by NESTLE using the intra-nodal cross sections are shown in Figure 4-11 through Figure 4-14. Note that the errors in fast group fluxes introduced by using flat cross sections is small and the errors in thermal group fluxes increase as burnup increases. The maximum percentage

Figure 4-10. Flux Shape by NESTLE Using $\Sigma^{(Intra)}_{xg}(x, y)$ at Bu=20 GWD/THM.
difference in the thermal flux at BOL is about -0.9% in LEU and -0.8% in MOX. However the maximum percentage difference in the thermal flux at a burnup of 20 GWD/THM reaches 3.2% in LEU and 3.9% in MOX at the edges of the node, i.e. the interface of the LEU and MOX fuel assemblies. The large percentage difference at the higher burnup level is due to the combined instantaneous interfacial effect and history effect, which is reflected in the much larger spatial variation of some of the intra-nodal cross sections, a behavior ignored when using the ‘flat’ cross sections.

Figure 4-11. Rel. Diff. in Flux by NESTLE at BOL (CS vs. Intra).

Figure 4-12. Rel. Diff. in Flux by NESTLE at Bu=0.5 GWD/THM (CS vs. Intra).

Figure 4-13. Rel. Diff. in Flux by NESTLE at Bu=10 GWD/THM (CS vs. Intra).

The percentage difference in the CS intra-nodal flux calculated by NESTLE using the node averaged cross sections from SA transport calculation with respect to the values by NESTLE using the intra-nodal cross sections are shown in Figure 4-15 through . Note that the errors in the fast group fluxes introduced by the flat cross section generated with the wrong spectra are still small (all less than 1%), although they increase with burnup increasing. The errors in the thermal group flux in the MOX fuel assembly increase with burnup increasing. The maximum percentage difference in thermal flux is about 0.5% at BOL and reaches 12% at

Figure 4-14. Rel. Diff. in Flux by NESTLE at Bu=20 GWD/THM (CS vs. Intra).

20 GWD/THM. It is interesting that the errors in the thermal group flux in the LEU fuel assembly do not always increase with burnup increasing. At a low burnup level they increase; at mid burnup level they decrease; and at high burnup level they increase again. The maximum relative difference is about 3.3% at BOL and reaches 7% at 500MWD/THM. However, the maximum relative difference decreases to about 0.8% at 10 GWD/THM and increases again to 6% at 20 GWD/THM. No matter how the maximum relative difference changes with burnup, it always occurs at the edges of the node, i.e. the interface of the LEU and MOX fuel assemblies. Contrasting errors with those obtained using ‘flat’ CS cross sections, the errors in ‘flat’ SA cross sections are larger with respect to ‘flat’ CS cross section. More evidence can be found by comparing the errors in $k_{\text{eff}}$ by the ‘flat’ CS and SA cross sections with respect to the intra-nodal cross section (see Table 4.1). The SA cross sections contribute larger errors to $k_{\text{eff}}$ than CS cross sections.

### Table 4.1: Errors in $k_{\text{eff}}$ by ‘Flat’ Cross Sections

<table>
<thead>
<tr>
<th>XS</th>
<th>0 GWD/THM</th>
<th>0.5GWD/THM</th>
<th>10GWD/THM</th>
<th>20GWD/THM</th>
</tr>
</thead>
<tbody>
<tr>
<td>CA</td>
<td>-1.2339e-4</td>
<td>-2.6324e-4</td>
<td>-2.5162e-4</td>
<td>-1.5830e-4</td>
</tr>
<tr>
<td>SA</td>
<td>1.7197e-3</td>
<td>2.8478e-3</td>
<td>1.5531e-3</td>
<td>-1.3409e-3</td>
</tr>
</tbody>
</table>
Figure 4-15. Rel. Diff. in Flux by NESTLE at BOL (SA vs. Intra).

Figure 4-16. Rel. Diff. in Flux by NESTLE at Bu=0.5 GWD/THM (SA vs. Intra).

Figure 4-17. Rel. Diff. in Flux by NESTLE at Bu=10 GWD/THM (SA vs. Intra).

CHAPTER 4: TRUE INTRA-NODAL FLUX

The accuracy of the intra-nodal flux distribution is very important to pin-wise power reconstruction. From the above figures, we can see how the flat cross sections impact the intra-nodal flux distribution. Even the flat cross sections collapsed with the correct spectra (the node-averaged cross sections obtained from CS transport calculation) will introduce errors into the intra-nodal flux. Hence it is necessary to utilize the spectrally correct, intra-nodal cross sections when completing the mixed LEU-MOX core simulation.

Figure 4-18. Rel. Diff. in Flux by NESTLE at Bu=20 GWD/THM (SA vs. Intra).


The accuracy of the intra-nodal flux distribution is very important to pin-wise power reconstruction. From the above figures, we can see how the flat cross sections impact the intra-nodal flux distribution. Even the flat cross sections collapsed with the correct spectra (the node-averaged cross sections obtained from CS transport calculation) will introduce errors into the intra-nodal flux. Hence it is necessary to utilize the spectrally correct, intra-nodal cross sections when completing the mixed LEU-MOX core simulation.
4.3. Comparison of Intra-nodal Flux

In this section, the intra-nodal flux obtained from diffusion (NESTLE) and transport (HELIOS) calculations for the LEU and MOX fuel assemblies is compared at several burnup levels, i.e. BOL, 0.5, 10 and 20 GWD/THM. Figure 4-19 through Figure 4-30 display the ratio in the CS intra-nodal flux as obtained from the diffusion and transport calculations for the LEU and MOX lattices using either the CS intra-nodal, CS flat or SA flat cross sections in the diffusion calculations.

Figure 4-19. Ratio of Intra-nodal Flux at BOL (Intra XS).

Figure 4-20. Ratio of Intra-nodal Flux at Bu=0.5 GWD/THM (Intra XS).

Figure 4-21. Ratio of Intra-nodal Flux at Bu=10 GWD/THM (Intra XS).

Figure 4-22. Ratio of Intra-nodal Flux at Bu=20 GWD/THM (Intra XS).

Figure 4-23. Ratio of Intra-nodal Flux at BOL (CS XS).

Figure 4-24. Ratio of Intra-nodal Flux at Bu=0.5 GWD/THM (CS XS).

Figure 4-25. Ratio of Intra-nodal Flux at Bu=10 GWD/THM (CS XS).

Figure 4-26. Ratio of Intra-nodal Flux at Bu=20 GWD/THM (CS XS).

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Figure 4-27. Ratio of Intra-nodal Flux at BOL (SA XS).

Figure 4-28. Ratio of Intra-nodal Flux at Bu=0.5 GWD/THM (SA XS).

Figure 4-29. Ratio of Intra-nodal Flux at Bu=10 GWD/THM (SA XS).

Referring to Eq. (2-21), we note that any difference in the intra-nodal flux as determined by the diffusion versus transport calculations translates into differences in the reconstructed heterogeneous flux, hence pin-powers in pin-power reconstruction. Ratios substantially different than unity, specially in the thermal group, can be observed at the edges of the lattice about the LEU-MOX interfaces. This effect is observed to be more pronounced in the MOX lattice at higher burnups. Compared with the transport solution, the maximum fast group flux errors by the diffusion solution for the three sets of cross sections are all quite small: about 0.5% in the LEU fuel assembly and 1% in the MOX fuel assembly at BOL. It is

Figure 4-30. Ratio of Intra-nodal Flux at Bu=20 GWD/THM (SA XS).

interesting to note that the maximum fast group flux error for the case when intra-nodal cross section are used decreases to 0.24% in the LEU fuel assembly and 0.45% in the MOX fuel assembly at 20 GWD/THM. These errors for the cases when ‘flat’ cross sections are used increase to 0.6% in the LEU fuel assembly but almost do not change in the MOX fuel assembly at 20 GWD/THM. The maximum thermal group flux errors in the LEU fuel assembly at BOL are about 3% for the cases when intra-nodal or CS cross sections are used and 5.9% for the case when SA cross section are used. The errors at the higher burnup level of 20 GWD/THM reach 0.9% for the case when intra-nodal cross sections are used, 3.7% for the case when CS cross sections are used and 6.1% for the case when SA cross sections are used. The maximum thermal group flux errors in the MOX fuel assembly at BOL are about 3.8% for all three cases. These errors at the higher burnup level of 20 GWD/THM reach 2% for the case when intra-nodal cross sections are used, 4% for the case when CS cross sections are used, and 10.7% for the case when SA cross sections are used. It is important to note how effective the utilization of intra-nodal cross sections is to improve the agreement between the diffusion theory and transport theory based determinations of the intra-nodal flux.
5. Power Form Factor

5.1. Power Form Factor

The form factor also plays an important role in the dehomogenization process. In practice, the form factors are obtained from the SA lattice calculation. No study has been found about the accuracy of the power form factor with regard to pin-wise power reconstruction for the mixed LEU-MIX core except one addressing the introduction of a group dependent form factor. From [4], the group form factors were shown to modestly improve the accuracy of predicting the pin-wise power distribution. In the current study, we address how much error there is in the form factors obtained from the traditional approach using SA lattice calculations.

The strategy for the study is described as follows:
1. Solve the diffusion equation for \( \Phi_g^{(\text{Intra})}(x, y) \) using \( \Sigma_{xy}^{(\text{Intra})}(x, y) \),
2. Evaluate the ratio of the exact group dependent power form factor, \( (f_g^P)^{(\text{Exact})} \), and approximate SA form factors, \( (f_g^P)^{(\text{SA})} \) as follows:
   \[
   \left( \frac{(f_g^P(x, y))^{(\text{Exact})}}{(f_g^P(x, y))^{(\text{SA})}} \right), \quad (5-1)
   \]
   where
   \[
   (f_g^P(x, y))^{(\text{Exact})} = \frac{\kappa \Sigma_{fg}^{(CS)}(x, y) \Phi_g^{(CS)}(x, y)}{\kappa \Sigma_{fg}^{(Intra)}(x, y) \Phi_g^{(Intra)}(x, y)}, \quad (5-2)
   \]
   \[
   (f_g^P(x, y))^{(\text{SA})} = \frac{\kappa \Sigma_{fg}^{(SA)}(x, y) \Phi_g^{(SA)}(x, y)}{\langle \kappa \Sigma_{fg}^{(SA)} \rangle \langle \Phi_g^{(SA)} \rangle}. \quad (5-3)
   \]

Figure 5-1 through Figure 5-4 display the ratio defined by Eq. (5-1), which shows the errors, i.e. deviations from 1.0, in the group dependent power form factor due to ignoring the interfacial effects. Huge interfacial effects can be observed in the thermal group power form factor at the edge of the nodes. These effects become smaller with burnup increasing. It is conjectured that more plutonium is burned than uranium during the burnup because of the difference in the power distribution (the power in MOX fuel assembly is higher than that in LEU fuel assembly), hence the differences in the properties of the LEU and MOX fuel assemblies becomes smaller as burnup increases. It follows that the interfacial effects become smaller with burnup increasing.
Figure 5-1. Ratio of Exact and SA Group Dependent Power FF at BOL.
Figure 5-2. Ratio of Exact and SA Group Dependent Power FF at Bu=0.5 GWD/THM
Figure 5-3. Ratio of Exact and SA Group Dependent Power FF at Bu=10 GWD/THM.
5.2. Discontinuity Factor

Another quantity we are concerned with is the discontinuity factor (DF): surface averaged DF (ADF) and corner point DF (CPDF). Since some of the DFs are defined right on the interface between LEU and MOX, the interfacial effect will no doubt impact them. DFs are employed not only in pin-wise power reconstruction, but also in solving the diffusion
equation by nodal methods, so selected to attempt to preserve the surface averaged currents. Hence they impact not only the nodal solution, but also the reconstruction. Thus it is quite important to analyze the accuracy of DFs for mixed LEU-MOX cores.

Figure 5-5 and Figure 5-6 show the heterogeneous flux values at BOL calculated by HELIOS CS calculation. The values of surface averaged, node averaged and corner point fast group fluxes show that the intra-nodal flux is flat in the LEU and MOX fuel assembly at BOL. However, those same values for the thermal group flux greatly differ.

<table>
<thead>
<tr>
<th>LEU</th>
<th>MOX</th>
</tr>
</thead>
<tbody>
<tr>
<td>CP flux</td>
<td></td>
</tr>
<tr>
<td>surface flux</td>
<td>node ave. flux</td>
</tr>
<tr>
<td>MOX</td>
<td>LEU</td>
</tr>
</tbody>
</table>

Figure 5-5. Exact Heterogeneous Fast Flux at BOL from HELIOS.
### 5.2.1 Surface Averaged Discontinuity Factor

The relative errors in the SA HELIOS determined ADFs are obtained by contrasting those values with the exact values obtained using NESTLE and CS HELIOS results, with NESTLE results obtained using intra-nodal cross sections. Mathematically, they are obtained as follows:

**Figure 5-6.** Exact Heterogeneous Thermal Flux at BOL from HELIOS.

<table>
<thead>
<tr>
<th>LEU</th>
<th>MOX</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.9013E-02</td>
<td>1.4990E-02</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LEU</th>
<th>MOX</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.4990E-02</td>
<td>1.3756E-02</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LEU</th>
<th>MOX</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0580E-02</td>
<td>1.0085E-02</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LEU</th>
<th>MOX</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0576E-02</td>
<td>1.0085E-02</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LEU</th>
<th>MOX</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.3197E-03</td>
<td>6.4239E-03</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LEU</th>
<th>MOX</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.8990E-03</td>
<td>6.3197E-03</td>
</tr>
</tbody>
</table>
\[ ADF_g^{(\text{Exact})} = \left\langle \phi_g^{(CS)} \right\rangle_{\text{Surface}} / \left\langle \phi_g^{(\text{Intra-Diff})} \right\rangle_{\text{Surface}}, \]  

(5-4)

and

\[ ADF_g^{(SA)} = \left\langle \phi_g^{(SA)} \right\rangle_{\text{Surface}} / \left\langle \phi_g^{(SA)} \right\rangle_{\text{Node}}. \]  

(5-5)

Table 5.1 through Table 5.2 display the relative errors in ADFs in the LEU and MOX fuel assemblies at burnups of 0, 0.5, 10 and 20 GWD/THM. The errors for the fast group ADFs are small both in the LEU and MOX fuel assemblies. For the thermal group ADFs, about a 1.5% error is observed in the LEU fuel assembly and a 2.2% error is observed in the MOX fuel assembly at BOL.

Table 5.1: Errors in ADFs in LEU.

<table>
<thead>
<tr>
<th>Group</th>
<th>Fast</th>
<th>Thermal</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Exterior</td>
<td>Interior</td>
</tr>
<tr>
<td>Sol.</td>
<td>BU=0</td>
<td></td>
</tr>
<tr>
<td>Exact</td>
<td>1.002134</td>
<td>0.997784</td>
</tr>
<tr>
<td>SA</td>
<td>1.00105</td>
<td>0.998793</td>
</tr>
<tr>
<td>Rel. Err.</td>
<td>-0.001081</td>
<td>0.001011</td>
</tr>
</tbody>
</table>
In practice, only the ratio of ADFs comes into play in the nodal solution and reconstruction. As shown in Table 5.3 and Table 5.4, the ratios of fast group ADFs are quite small for all the burnup levels. However about a 2.7% error is observed in the ratio of the thermal group ADFs at BOL and the errors become smaller with burnup.

### Table 5.2: Errors in ADFs in MOX.

<table>
<thead>
<tr>
<th>Group</th>
<th>Fast</th>
<th></th>
<th>Thermal</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Sol.</td>
<td>Exterior</td>
<td>Interior</td>
<td>Exterior</td>
</tr>
<tr>
<td>Bu=0</td>
<td>Exact</td>
<td>0.993974</td>
<td>1.002609</td>
<td>1.10052</td>
</tr>
<tr>
<td></td>
<td>SA</td>
<td>0.996954</td>
<td>1.00111</td>
<td>1.12499</td>
</tr>
<tr>
<td></td>
<td>Rel. Err.</td>
<td>0.002998</td>
<td>-0.001495</td>
<td>0.022235</td>
</tr>
<tr>
<td>Bu=0.5GWD/THM</td>
<td>Exact</td>
<td>0.99406</td>
<td>1.002583</td>
<td>1.107859</td>
</tr>
<tr>
<td></td>
<td>SA</td>
<td>0.996877</td>
<td>1.00116</td>
<td>1.12498</td>
</tr>
<tr>
<td></td>
<td>Rel. Err.</td>
<td>0.002834</td>
<td>-0.001419</td>
<td>0.015454</td>
</tr>
<tr>
<td>Bu=10GWD/THM</td>
<td>Exact</td>
<td>0.995353</td>
<td>1.002266</td>
<td>1.101343</td>
</tr>
<tr>
<td></td>
<td>SA</td>
<td>0.996839</td>
<td>1.00144</td>
<td>1.11137</td>
</tr>
<tr>
<td></td>
<td>Rel. Err.</td>
<td>0.001493</td>
<td>-0.000824</td>
<td>0.009105</td>
</tr>
<tr>
<td>Bu=20GWD/THM</td>
<td>Exact</td>
<td>0.996191</td>
<td>1.002171</td>
<td>1.082083</td>
</tr>
<tr>
<td></td>
<td>SA</td>
<td>0.997119</td>
<td>1.00138</td>
<td>1.09447</td>
</tr>
<tr>
<td></td>
<td>Rel. Err.</td>
<td>0.000932</td>
<td>-0.000789</td>
<td>0.011447</td>
</tr>
</tbody>
</table>

### Table 5.3: Errors in Ratio of Fast ADFs

<table>
<thead>
<tr>
<th>BU(GWD/THM)</th>
<th>0</th>
<th>0.5</th>
<th>10</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exact</td>
<td>0.991857</td>
<td>0.991812</td>
<td>0.993062</td>
<td>0.993311</td>
</tr>
<tr>
<td>SA</td>
<td>0.995908</td>
<td>0.995801</td>
<td>0.995386</td>
<td>0.995029</td>
</tr>
<tr>
<td>Rel. Err.</td>
<td>0.00408</td>
<td>0.00402</td>
<td>0.00234</td>
<td>0.0017</td>
</tr>
</tbody>
</table>

Note: $Ratio = (ADF_g)^{MOX}/(ADF_g)^{LEU}$
How much will the errors in the ADFs effect the accuracy of the predicted values of $k_{\text{eff}}$, node averaged fluxes, fuel assembly surface currents and intra-nodal fluxes? To address this problem, a color set fine mesh calculation was performed by NESTLE using the nodal method with the ADFs distribution imposed along the interface between the LEU and MOX fuel assemblies. The ADFs distribution along the interface is calculated by Eq. (5-4) using the heterogeneous flux obtained from HELIOS and homogeneous flux obtained from NESTLE at each surface segment. Six cases were performed for this study: intra-nodal cross sections and exact ADFs are used in case 1, intra-nodal cross sections and SA ADFs are used in case 2, CS cross sections and exact ADFs are used in case 3, CS cross sections and SA ADFs are used in case 4, SA cross sections and exact ADFs are used in case 5, and SA cross sections and SA ADFs are used in case 6.

Table 5.5 shows the errors in $k_{\text{eff}}$ for each case. It shows that ADFs do not greatly effect the $k_{\text{eff}}$ value. The main error source comes from the cross sections, i.e. the energy and spatial spectrum used for generating the cross sections. Likewise the ADFs do not impact much the node averaged fluxes.

Table 5.4: Errors in Ratio of Thermal ADFs

<table>
<thead>
<tr>
<th>BU (GWD/THM)</th>
<th>0</th>
<th>0.5</th>
<th>10</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exact</td>
<td>1.117982</td>
<td>1.147574</td>
<td>1.145315</td>
<td>1.135572</td>
</tr>
<tr>
<td>SA</td>
<td>1.148637</td>
<td>1.148283</td>
<td>1.142079</td>
<td>1.133256</td>
</tr>
<tr>
<td>Rel. Err.</td>
<td>0.0274</td>
<td>0.00062</td>
<td>-0.0028</td>
<td>-0.002</td>
</tr>
</tbody>
</table>

Note: $Ratio = \frac{(ADF_g)^{\text{MOX}}}{(ADF_g)^{\text{LEU}}}$
Table 5.5: Errors in $k_{\text{eff}}$

<table>
<thead>
<tr>
<th>BU (GWD/THM)</th>
<th>0</th>
<th>0.5</th>
<th>10</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ref. $k_{\text{eff}}$</td>
<td>1.29671</td>
<td>1.25362</td>
<td>1.15254</td>
<td>1.07389</td>
</tr>
<tr>
<td>Case 1</td>
<td>1.3881e-5</td>
<td>-1.6751e-5</td>
<td>-2.5769e-5</td>
<td>-2.2349e-5</td>
</tr>
<tr>
<td>Case 2</td>
<td>3.8559e-5</td>
<td>-1.9145e-4</td>
<td>-4.5291e-5</td>
<td>-2.1874e-4</td>
</tr>
<tr>
<td>Case 3</td>
<td>8.0203e-5</td>
<td>-1.7007e-4</td>
<td>4.5725e-5</td>
<td>-9.0605e-5</td>
</tr>
<tr>
<td>Case 4</td>
<td>2.2827e-4</td>
<td>-1.9781e-4</td>
<td>6.4813e-5</td>
<td>-8.3807e-5</td>
</tr>
<tr>
<td>Case 5</td>
<td>1.1785e-3</td>
<td>1.3964e-3</td>
<td>2.4231e-3</td>
<td>2.2346e-3</td>
</tr>
<tr>
<td>Case 6</td>
<td>1.1969e-3</td>
<td>1.4213e-3</td>
<td>2.4441e-3</td>
<td>2.2486e-3</td>
</tr>
</tbody>
</table>

Note: Ref. $k_{\text{eff}}$ -- $k_{\text{eff}}$ obtained by HELIOS CS calculation.

- Case 1 -- calculation using intra-nodal cross sections and exact ADFs.
- Case 2 -- calculation using intra-nodal cross sections and SA ADFs.
- Case 3 -- calculation using CS cross sections and exact ADFs.
- Case 4 -- calculation using CS cross sections and SA ADFs.
- Case 5 -- calculation using SA cross sections and exact ADFs.
- Case 6 -- calculation using SA cross sections and SA ADFs.

Figure 5-7 and Figure 5-8 show the currents at the interface between the LEU and MOX fuel assemblies. The interface is located at the east side of the LEU fuel assembly and the west side of the MOX fuel assembly. Cell 1 in the figures indicates the most north cell, implying the highest numbered cell is adjacent to the point where the 4 assemblies form a common corner. The ADFs along with the cross sections do impact the shape of the current distribution, especially for the cell out half an assembly pitch from the common corner. Note how effective the usage of intra-nodal cross sections are in obtaining the correct surface current, *i.e.* leakage.
Figure 5-7. Comparison of Fast Surface Current at LEU-MOX Interface.
Figure 5-8. Comparison of Thermal Surface Current at LEU-MOX Interface.
The relative error distributions of the group dependent intra-nodal fluxes are shown in Figure 5-9 through Figure 5-32 for the six cases at burnups of 0, 0.5, 10 and 20 GWD/THM. The errors are determined with reference to the CS determined intra-nodal flux. The errors in the fluxes are due to the method, cross sections and the ADFs. Table 5.6 summarizes the maximum errors of the fuel pin average fluxes and water gap fluxes as a function of burnup and assembly type for each case. Table 5.7 summarizes the maximum errors of the fuel pin average fluxes as a function of burnup and assembly type for each case.

Table 5.6: Maximum Relative Errors for the Intra-nodal Fluxes

<table>
<thead>
<tr>
<th>Burnup (GWD/THM)</th>
<th>Case</th>
<th>Intra-nodal Flux Maximum Error (%)</th>
<th>LEU</th>
<th>MOX</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Group 1</td>
<td>Group 2</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0.0028</td>
<td>0.0206</td>
<td>0.0031</td>
</tr>
<tr>
<td>0</td>
<td>2</td>
<td>0.6005</td>
<td>1.5295</td>
<td>0.2610</td>
</tr>
<tr>
<td>0</td>
<td>3</td>
<td>0.0728</td>
<td>0.2702</td>
<td>0.0295</td>
</tr>
<tr>
<td>0</td>
<td>4</td>
<td>0.6432</td>
<td>1.7290</td>
<td>0.2396</td>
</tr>
<tr>
<td>0</td>
<td>5</td>
<td>0.0320</td>
<td>0.2693</td>
<td>0.0598</td>
</tr>
<tr>
<td>0</td>
<td>6</td>
<td>0.6013</td>
<td>1.5487</td>
<td>0.2723</td>
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Table 5.7: Maximum Relative Errors for the Fuel Pin Average Fluxes

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Figure 5-9. Rel. Error of Flux at BOL (Case 1).
Figure 5-10. Rel. Error of Flux at Bu=0.5 GWD/THM (Case 1).
Figure 5-11. Rel. Error of Flux at Bu=10 GWD/THM (Case 1).
Figure 5-12. Rel. Error of Flux at $Bu=20$ GWD/THM (Case 1).
Figure 5-13. Rel. Error of Flux at BOL (Case 2).
Figure 5-14. Rel. Error of Flux at Bu=0.5 GWD/THM (Case 2).
Figure 5-15. Rel. Error of Flux at Bu=10 GWD/THM (Case 2).
Figure 5-16. Rel. Error of Flux at Bu=20 GWD/THM (Case 2).
Figure 5-17. Rel. Error of Flux at BOL (Case 3).
Figure 5-18. Rel. Error of Flux at $Bu=0.5$ GWD/THM (Case 3).
Figure 5-19. Rel. Error of Flux at Bu=10 GWD/THM (Case 3).
Figure 5-20. Rel. Error of Flux at Bu=20 GWD/THM (Case 3).
Figure 5-21. Rel. Error of Flux at BOL (Case 4).
Figure 5-22. Rel. Error of Flux at Bu=0.5 GWD/THM (Case 4).
Figure 5-23. Rel. Error of Flux at Bu=10 GWD/THM (Case 4).
Figure 5-24. Rel. Error of Flux at Bu=20 GWD/THM (Case 4).
Figure 5-25. Rel. Error of Flux at BOL (Case 5).
Figure 5-26. Rel. Error of Flux at Bu=0.5 GWD/THM (Case 5).
Figure 5-27. Rel. Error of Flux at Bu=10 GWD/THM (Case 5).
Figure 5-28. Rel. Error of Flux at Bu=20 GWD/THM (Case 5).
Figure 5-29. Rel. Error of Flux at BOL (Case 6).
Figure 5-30. Rel. Error of Flux at Bu=0.5 GWD/THM (Case 6).
Figure 5-31. Rel. Error of Flux at Bu=10 GWD/THM (Case 6).
5.2.2 Corner Point Discontinuity Factor

The CPDFs are utilized in pin-wise power reconstruction. The accuracy of this quantity will impact the accuracy of the flux near the corner point. As was done with ADFs, the exact and SA determined values of CPDFs are evaluated. The relative errors in CPDFs are shown in Table 5.8 through Table 5.11. Note that the NW in the tables indicates the point of the fuel assembly center, and SE indicates the point of the checkerboard center. Similar with ADFs, the errors in the fast group CPDFs are small both in the LEU and MOX fuel assemblies. About a 3% error is observed in the thermal group CPDFs in the LEU fuel assembly at BOL which reduces to 1.2% at a burnup of 20 GWD/THM. About a 4.4% error is
observed in the MOX fuel assembly at BOL which reduces to 2.4% at a burnup of 20 GWD/THM.

Table 5.8: Errors in Fast CPDFs in LEU.

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Table 5.9: Errors in Thermal CPDFs in LEU.

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Table 5.10: Errors in Fast CPDFs in MOX.

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Table 5.11: Errors in Thermal CPDFs in MOX.

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</tr>
<tr>
<td>Exact</td>
<td>1.100065</td>
<td>1.126990</td>
<td>0.024476</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.27332</td>
<td>1.282700</td>
<td>0.007366</td>
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</tr>
<tr>
<td></td>
<td>1.100066</td>
<td>1.126980</td>
<td>0.024466</td>
<td></td>
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<tr>
<td></td>
<td>1.47766</td>
<td>1.477610</td>
<td>-0.000034</td>
<td></td>
</tr>
</tbody>
</table>
To address how the CPDFs introduce the errors to the corner point fluxes, Smith’s method is used to evaluate the relative errors in the homogeneous flux at the LEU-MOX interface corner points, i.e., checkerboard center and out half an assembly pitch, with the exact intra-nodal flux corner point flux and CPDFs which have errors. Table 5.12 and Table 5.13 show the relative errors in the corner points (NE and SE) flux.

<table>
<thead>
<tr>
<th>Table 5.12: Relative Errors in CP Fluxes in LEU</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Bu(}\text{GWD/THM}) )</td>
</tr>
<tr>
<td>NE_fast</td>
</tr>
<tr>
<td>SE_fast</td>
</tr>
<tr>
<td>NE_thermal</td>
</tr>
<tr>
<td>SE_thermal</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 5.13: Relative Errors in CP Fluxes in MOX</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Bu(}\text{GWD/THM}) )</td>
</tr>
<tr>
<td>NE_fast</td>
</tr>
<tr>
<td>SE_fast</td>
</tr>
<tr>
<td>NE_thermal</td>
</tr>
<tr>
<td>SE_thermal</td>
</tr>
</tbody>
</table>

5.3. Node Averaged Reaction Rates

As discussed in chapter 2, we need to know \( \Sigma_{xg}^{\text{(Intra)}}(x, y) \) in order to accurately solve the diffusion equation. But the reaction rate preserving normalization factor depends upon \( \phi_{g}^{\text{(Intra)}}(x, y) \), which should be based upon the diffusion equation solution. Hence, we are into a circular argument. In this study, the intra-nodal cross sections are determined using CS and SA lattice calculations as defined; then the diffusion equation is solved for the intra-nodal flux using these intra-nodal cross sections. Note that
because of the normalization factor containing a small error. How large the errors in the reaction rates are due to the normalization factor errors is shown in Table 5.14 and Table 5.15, which presents the ratios of the reaction rates defined as follows:

\[
\text{Ratio} = \frac{\iint \sum_{xg}^{(Intra)}(x, y)\phi_g^{(Intra)}(x, y) dy dx}{\iint \sum_{xg}^{(CS)}(x, y)\phi_g^{(CS)}(x, y) dy dx}
\]  

\(5-7\)

Table 5.14: Ratio of Reaction Rates in LEU.

<table>
<thead>
<tr>
<th>bu</th>
<th>0</th>
<th>0.5G</th>
<th>10G</th>
<th>20G</th>
</tr>
</thead>
<tbody>
<tr>
<td>tr1</td>
<td>0.999988</td>
<td>1.000005</td>
<td>0.999966</td>
<td>1.0000171</td>
</tr>
<tr>
<td>ab1</td>
<td>0.999931</td>
<td>1.000061</td>
<td>1.000089</td>
<td>0.9999213</td>
</tr>
<tr>
<td>nf1</td>
<td>1.000007</td>
<td>1.000005</td>
<td>1.000011</td>
<td>0.9999905</td>
</tr>
<tr>
<td>s12</td>
<td>0.999952</td>
<td>0.999989</td>
<td>1.000044</td>
<td>0.9999021</td>
</tr>
<tr>
<td>tr1</td>
<td>1.000002</td>
<td>0.999904</td>
<td>1.000041</td>
<td>1.0000314</td>
</tr>
<tr>
<td>ab2</td>
<td>1.000019</td>
<td>0.999930</td>
<td>0.999946</td>
<td>1.0000516</td>
</tr>
<tr>
<td>nf2</td>
<td>1.000029</td>
<td>0.999967</td>
<td>1.000036</td>
<td>0.9999928</td>
</tr>
</tbody>
</table>

Table 5.15: Ratio of Reaction Rates in MOX.

<table>
<thead>
<tr>
<th>bu</th>
<th>0</th>
<th>0.5G</th>
<th>10G</th>
<th>20G</th>
</tr>
</thead>
<tbody>
<tr>
<td>tr1</td>
<td>0.999976</td>
<td>0.999964</td>
<td>1.000042</td>
<td>1.0000211</td>
</tr>
<tr>
<td>ab1</td>
<td>0.999888</td>
<td>0.999999</td>
<td>0.999968</td>
<td>0.9999135</td>
</tr>
<tr>
<td>nf1</td>
<td>0.999998</td>
<td>0.999982</td>
<td>1.000012</td>
<td>0.9999827</td>
</tr>
<tr>
<td>s12</td>
<td>0.999875</td>
<td>0.999999</td>
<td>1.000053</td>
<td>0.9999661</td>
</tr>
<tr>
<td>tr1</td>
<td>0.999935</td>
<td>0.999988</td>
<td>1.000057</td>
<td>1.0000265</td>
</tr>
<tr>
<td>ab2</td>
<td>0.999975</td>
<td>0.999933</td>
<td>1.000055</td>
<td>1.0000405</td>
</tr>
<tr>
<td>nf2</td>
<td>0.999986</td>
<td>0.999978</td>
<td>1.000087</td>
<td>1.0000364</td>
</tr>
</tbody>
</table>

The ratios of the reaction rates for the LEU and MOX fuel assemblies are very close to unity, indicating that the normalization factor errors are of no consequence.
6. Summary and Future Work

The study of the true intra-nodal cross section and flux is completed using results from SA and CS lattice physics calculations (HELIOS), and diffusion calculations (NESTLE) using the finite difference method with surface currents obtained from the CS calculation as the boundary condition.

Large relative differences are observed in several types of node-averaged (homogenized) cross sections as determined by HELIOS SA calculations versus those determined by HELIOS CS calculations, particularly in the thermal group cross sections. Even the thermal group diffusion coefficient shows appreciable difference, this interfacial induced change believed ignored in currently employed methods. Local spectrum plays a very important role in the homogenization process. A CS calculation for each possible checkerboard is impractical during fuel management calculations. How to use the cross sections from SA calculations to get acceptable accurate cross sections is an open issue. Rehomogenization for the cross sections obtained from the SA lattice calculation becomes necessary for the mixed LEU-MOX core simulation. The spectra correction proposed by Kord Smith may be a solution to this problem.

Regarding the spatial shape of the intra-nodal cross sections, stronger spatial dependence is observed for the down-scatter, thermal absorption, and fast and thermal fission cross sections. With regard to stronger dependence on burnup, the same cross section types as identified for stronger spatial dependence are involved. No doubt, the shape of intra-nodal cross section shows that the thermal group “flat” cross section cannot represent the interfacial effect. This assumption no longer works for mixed LEU-MOX cores. Note that the spatial distribution at BOL is totally due to instantaneous intra-nodal spectra effects since no fuel depletion has yet taken place. The spatial distributions with burnup are due to not only instantaneous intra-nodal spectral effects, but also the history (cumulative) impact on the spatial distributions of the nuclei isotopes due to intra-nodal effects. The issue of how to spatially functionalize the intra-nodal cross sections has not yet been addressed, but likely will not be adequately done using a lower order separable in x and y polynomial because of the strong spatial behavior in the unit cells located two deep from the LEU-MOX lattice interfaces. Also, where the values that the functionalized cross sections will be fitted to remains an open issue.

Generally, the surface averaged cross sections, used as constraints in spatially functionalizing intra-nodal cross sections, are obtained by interpolating to the surface averaged burnup level using the node averaged cross section information from SA
calculations. The solution from this traditional approach is compared with the values obtained by averaging the surface intra-nodal cross sections at the surface burnup level, which is evaluated by linearly extrapolating from nearby adjacent nodes. There are two open issues in evaluating the surface cross sections. One is how to accurately predict the surface burnup level? Another is how to rehomogenized the surface cross section to take into account the interfacial effect? A high order polynomial is recommended for pin-wise burnup reconstruction.

The CS intra-nodal flux shapes calculated by NESTLE utilizing the fine-mesh finite different method with the intra-nodal cross sections display steep thermal flux gradients at the edges of the node, i.e. the interface of the LEU and MOX lattices. The resulting flux shape presents a difficult problem to accurately functionalize.

A study on the relative difference in the CS intra-nodal flux calculated by NESTLE using node averaged cross sections from CS transport calculation with respect to the values by NESTLE using intra-nodal cross sections shows how much error the flat cross sections introduce to the intra-nodal flux. The errors in the fast group fluxes introduced by the flat cross section are small (<1% for both the LEU and MOX fuel assembly), whereas the errors in the thermal group fluxes increase with the burnup increasing (~3.2% in the LEU fuel assembly and ~3.9% in the MOX fuel assembly).

A study on the relative difference in the CS intra-nodal flux calculated by NESTLE using node averaged cross sections from SA transport calculation with respect to the values by NESTLE using intra-nodal cross sections shows the error introduced by the SA cross sections without spatial shape. The errors in the fast group fluxes introduced by the flat SA cross sections are small (all less than 1%). The errors in the thermal group flux in the MOX fuel assembly increase with the burnup increasing (maximum error ~12%). It is interesting that the errors in the thermal group fluxes in the LEU fuel assembly do not always increase with the burnup increasing. Initially, it increases at low burnups, then decreases as burnup increases, and once again increases at higher burnups. No matter how the maximum error changes with burnup, it always occurs at the edges of the node, i.e. the interface of the LEU and MOX fuel assembly.

This study also shows how flat cross sections impact the accuracy of the predicted intra-nodal flux distribution. Even the flat cross sections collapsed with the correct spectra (the node-averaged cross section obtained from CS transport calculation) will introduce errors to the intra-nodal flux. This supports again that cross section rehomogenization and intra-nodal cross section are very important in mixed LEU-MOX core simulation.

More evidence can be found by comparing the errors in $k_{eff}$ by the ‘flat’ CS and SA
cross sections with respect to the intra-nodal cross sections. The SA cross sections contribute larger errors to $k_{\text{eff}}$ than CS cross sections: the maximum error contributed by CS cross sections is about 0.026% and that by SA cross sections is about 0.28%.

How to accurately evaluate the intra-nodal flux distribution is very important to pin-wise power reconstruction. The issue of how to spatially functionalize the intra-nodal flux has not yet been addressed, but likely will not be adequately done using a combination of polynomial and hyperbolic function forms because of the strong spatial behavior near the LEU-MOX lattice interfaces. Also, what values that the functionalized flux will be fitted to remains an open issue.

The intra-nodal fluxes from diffusion and transport solutions are compared at several burnup levels by calculating their ratio. Ratios much different than unity, specially in the thermal group, are observed at the edges of the lattice about the LEU-MOX interfaces. It is important to note how effective the utilization of intra-nodal cross sections are in improving the agreement between the diffusion theory and transport theory based determinations of the intra-nodal flux.

The form factor also plays an important role in the dehomogenization process. In practice, the form factors are obtained from the SA lattice calculation. This study analyzes the errors in the group dependent power form factor due to ignoring the interfacial effects. Large interfacial effects are observed in the thermal group power form factor at the edge of the nodes (maximum $\sim 10\%$). These effects becomes smaller and smaller with the burnup increasing. The group dependent form factors will improve the prediction accuracy of pin-wise powers, however, the improvement is limited. Is it necessary to correct the form factors for interfacial effects, but how to correct them, is an open issue.

Another quantity of concerned is the discontinuity factor (DF): both ADF and CPDF. Since for the outer assembly surface, they are defined right on the interface between the LEU and MOX fuel assemblies, the interfacial effect will no doubt impact them. ADFs appear in the nodal solution in the form of ratio of adjacent surfaces. Hence, we are concerned with the errors in the ADF ratios. The relative errors in the fast group ADF ratios are small (all less than 0.4%). However about a 2.7% relative error is observed in the thermal group ADFs’ ratios at BOL. The errors reduce with burnup increasing. Unlike ADFs, CPDFs are utilized in pin-wise power reconstruction. The errors in the fast group CPDFs are very small (all less than 1%). However larger errors in the thermal group CPDFs are observed in both the LEU and MOX fuel assemblies: about a 3% error in the LEU fuel assembly at BOL which reduces to 1.2% at a burnup of 20 GWD/THM and a 4.4% error in the MOX fuel assembly at BOL which reduces to 2.4% at a burnup of 20 GWD/THM. The accuracy of this quantity will impact the
flux shape near the corner point. How to correct DFs is an open issue to be addressed later.

The study on the effect of ADF’s and cross sections shows that errors in the cross sections, i.e. the energy and spatial spectrum used for generating the cross sections, are the main contributors to the $k_{eff}$, node averaged fluxes and intra-nodal fluxes. ADFs do not greatly effect the $k_{eff}$ value. Likewise the ADFs do not impact much the node averaged fluxes.

In conclusion, the work reported upon here will serve as a basis to provide benchmarks for approximate methods that only utilize SA lattice calculations to obtain the required cross section input to nodal based core simulators.
References


REFERENCES


