

# **An Assessment of Advanced Nodal Methods for MOX Fuel Analysis in Light Water Reactors**

T. Downar, C.H. Lee, G. Jiang  
School of Nuclear Engineering  
Purdue University  
downar@ecn.purdue.edu

## ***Abstract***

*There has been concern during the last several years that the advanced nodal methods which have been developed for LWR cores initially fueled with Uranium do not provide the same accuracy when applied to the same cores initially fueled with mixed oxide. Several modifications to the existing methods have been proposed and some have been implemented in utility and vendor codes. The purpose of this paper is to provide a framework for understanding some of the limitations in modern nodal methods and for examining some of the modifications available for improving the accuracy of nodal methods MOX fuel analysis.*

## **1.0 Introduction**

The current state of the art in reactor physics methods represents a long period of successful methods and code development. Core criticality and the fission power distribution of the current generation of LWRs can be very accurately predicted for the expected range of reactor operating conditions. During the past several years there has been some concern that the advanced nodal methods that have been developed for uranium fueled LWRs do not perform satisfactorily when applied to the same cores fueled with mixed oxide (MOX), or more generally to cores with very different neutron spectra.

The accuracy of the nodal solution is particularly important for the best estimate analysis of MOX fueled LWRs since the presence of MOX can exacerbate the kinetics response of the core. For example, the end of cycle moderator temperature coefficient will be more negative in a MOX fueled core, which will increase the positive reactivity insertion during a main steam line break event in a PWR. Also, the delayed neutron fraction in a MOX fueled core will be smaller and the energy deposition during a postulated rod ejection accident can increase. This makes it important that the accuracy of nodal methods for MOX fuel analysis are at least as accurate as methods used for the analysis of UO<sub>2</sub> fueled cores.

During the last decade, there has been considerable experience in both Europe and Japan with the irradiation of reactor grade MOX fuel. There has been extensive analysis of the operating data from these reactors, as well as numerous MOX critical experiments such as those at the VENUS facility in Belgium. Special workshops have been organized specifically to address MOX fuel issues such as the 1998 OECD Workshop in Paris on the "Physics and Fuel Performance of Reactor-Based Plutonium Disposition" [Sevelli, 1998].

The purpose of this paper is not to provide a review of the extensive literature on the physics and performance of MOX fuel. Rather, the objective of this paper is to provide a framework for understanding some of the limitations of advanced nodal methods for MOX fuel analysis, as well as some of the recent modifications designed to improve the accuracy of the codes for analyzing MOX fuel. The specific focus of this paper will be to assess the limitations of modern nodal methods used to predict the core eigenvalue and power distribution. Because nodal neutronics methods are frequently used in coupled thermal-hydraulics/spatial kinetics codes, this focus is most appropriate to assess the impact of MOX fuel on best estimate core safety analysis.

## 2.0 Core Neutronics Analysis Methods

The solution of the Boltzmann transport equation for computing the neutron flux and the reactor core power distribution in light water reactors is usually performed with a two step process. In the first step, the integral transport equation is solved for individual fuel assemblies with primary focus on the energy dependence of the neutron interactions. The result of this "lattice calculation" is a set of homogenized few group constants which are then used in the second step to solve the diffusion equation for the spatial flux distribution in the entire core. This process is depicted in Figure 1.

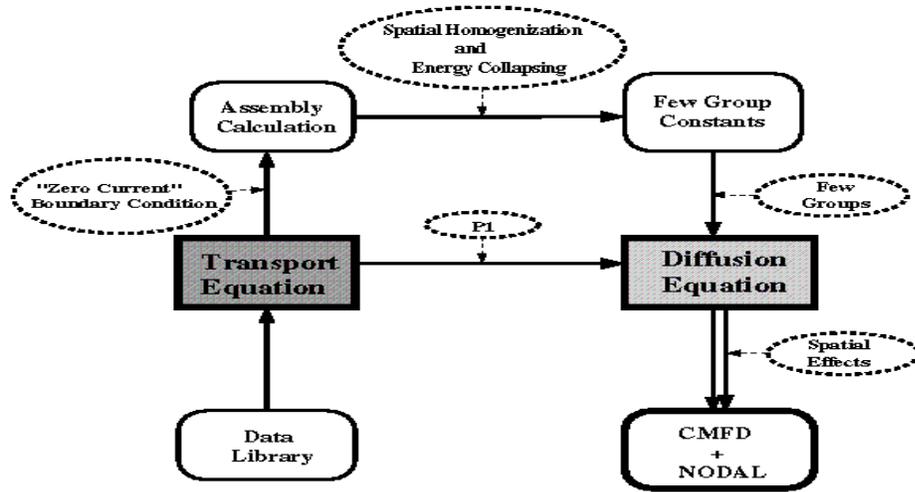


Figure 1 Modern Neutron Physics Solution Strategy

This two step method has proven successful for the analysis of Light Water Reactors fueled with enriched uranium dioxide fuel. The reactor core power distribution has consistently been predicted within a few percent of measurements. During the last several years there has been considerable discussion within the reactor physics community about which assumptions made in this solution strategy may be inappropriate for the analysis of MOX fuel. This discussion has generally focused separately on the limitations with group constant generation in the lattice physics codes and on the limitations of the nodal codes themselves. Several authors have noted some limitations in the group constant generation methods used for MOX fuel analysis [Edenius, 1998], [Finck, 1998], [Joo, 1999], [Nakdagym 1998]. The analysis here will be confined to the limitations in the advanced nodal codes.

### Modern Nodal Methods for MOX Fuel Analysis

Modern nodal methods have been widely used for the last several years to provide the core power distribution for both core depletion and transient analysis. The general consensus is that the deficiencies of the current methods for MOX fuel analysis can be isolated into four primary effects: (1) a homogenization effect, (2) a spatial discretization effect, (3) a group collapsing effect, and (4) a transport effect. Each of these effects will be briefly reviewed in the following section and demonstrated with a simple MOX benchmark problem.

#### *MOX Benchmark Problem*

A simple one-dimensional MOX benchmark problem can be useful to demonstrate the sources of inaccuracies in modern nodal methods for MOX fuel analysis. UO<sub>2</sub> (3 w/o) and MOX (8 w/o) fuel assemblies were placed adjacent to a water reflector region as shown below in Figure 2. A reflective boundary condition was imposed on all external interfaces to simplify the analysis.

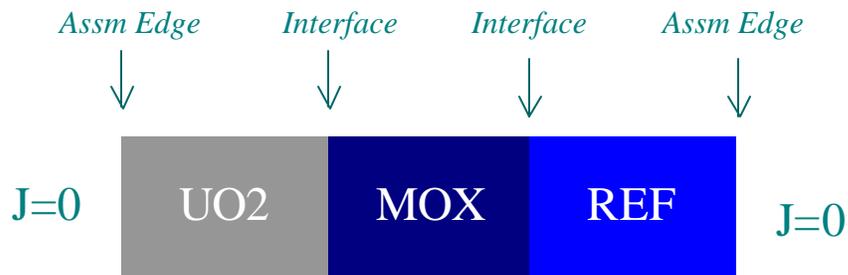


Figure 2 MOX Benchmark Problem

A 97 group multi-assembly “color set” calculation was performed on this problem with the lattice physics code CPM-03 [Jones, 97] and served as the reference for analyzing each of the

four effects. In order to graphically display the neutron flux shapes, the reference 97 group fluxes were integrated into 2 groups with the thermal group cut off at the standard 0.625 eV. The plots are shown in Figure 3. The fast flux distribution is smooth, but the thermal flux varies dramatically with significant gradients at both the UO<sub>2</sub>/MOX and MOX/REF interfaces.

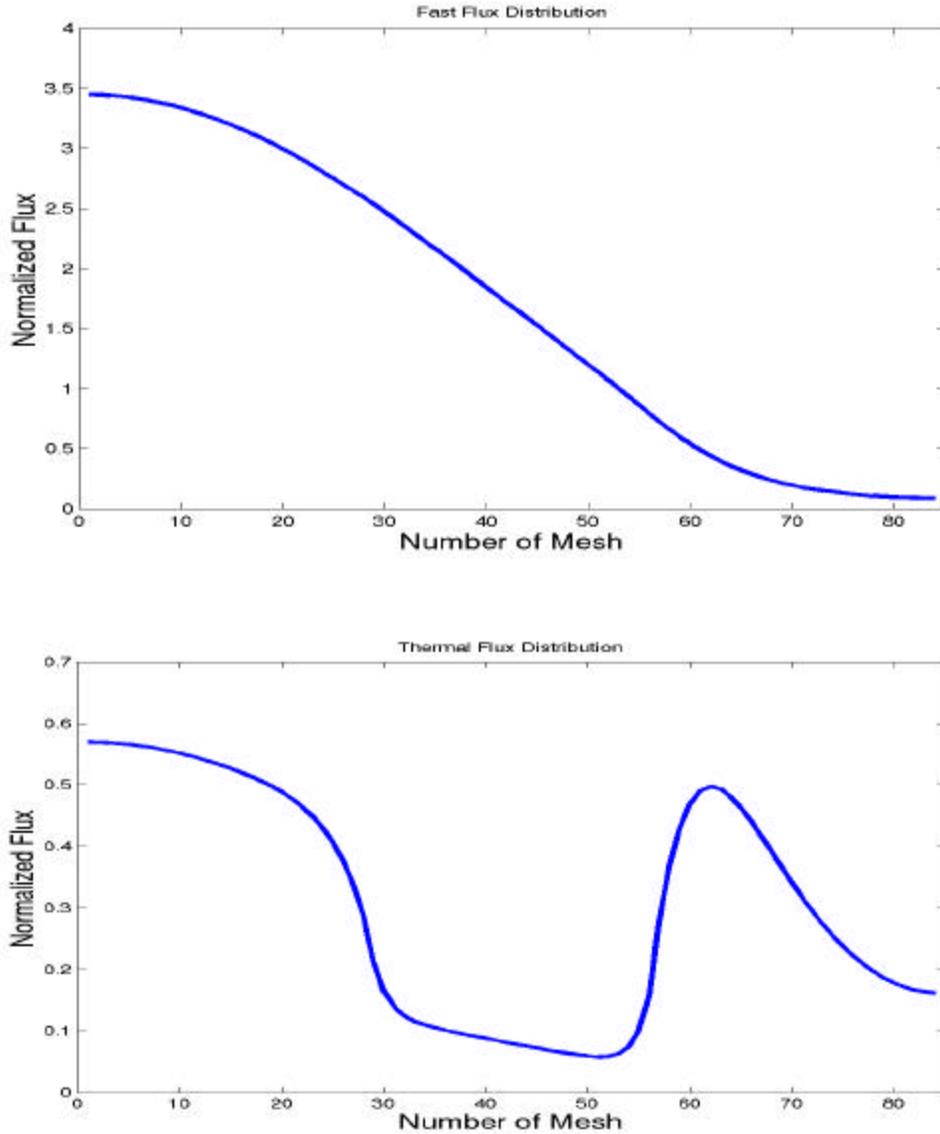


Figure 3 Fast and Thermal Flux Distributions in MOX Benchmark Problem

The following sequence of calculations were performed to isolate each of the effects indicated:

1. **Homogenization Effect:** A fine mesh finite difference diffusion solution with 97 group constants from a “zero current” boundary condition single assembly calculation.
2. **Spatial Discretization Effect:** A nodal diffusion solution with 2 group, single assembly group constants.
3. **Collapse Effect:** A fine mesh finite difference diffusion theory solution with single assembly group constants at 97, 8, 4, and 2 energy groups.
4. **Transport Effect:** A fine mesh finite difference P3 transport and diffusion (P1) solution with the exact 97 group constants.

The results of each of these calculations were compared to the CPM-03 “colorset” reference. It should be noted that this example only considers the assembly “homogenization effect” whereas additional homogenization error is introduced when homogenizing the fuel, cladding, and moderator at the pin cell level. Of these two homogenization effects, the assembly homogenization effect can be more important for predicting core behavior. Future studies will assess the impact of pin cell homogenization errors, although the recent work of Smith, et al. [Smith, 2000] suggests that this can also be an important effect.

### *The Homogenization Effect*

During the calculation of the assembly homogenized group constants, a zero current boundary condition is imposed on the fuel assembly. The group constants are then used in a core environment in which there is substantial leakage into and out of the fuel assembly. Strictly speaking, the group constants should then be recalculated with an updated estimate of the assembly boundary conditions. However, experience has shown that the error introduced with the zero current assumption is small for standard uranium dioxide fueled cores. Recently, several researchers have shown that the strong mismatch in flux spectra between uranium dioxide and mixed oxide fuel assemblies can lead to significant errors in the homogenized group constants.

The 97-group neutron spectra are shown in Figs. 4, 5, and 6 for the center of each assembly and the two interfaces. In the UO<sub>2</sub> assembly, the spectrum at the right surface is hardened because of the presence of the MOX fuel and therefore the spectrum is very similar to the spectrum at the left surface of the MOX assembly. The spectral interaction at the MOX/REF interface is even more pronounced. The spectrum at the right surface of the MOX fuel assembly is very soft and similar to the left surface spectrum of the reflector. The fast to thermal flux ratio is much lower because the magnitude of the fast neutron flux is about the same as the magnitude of the thermal neutron flux.

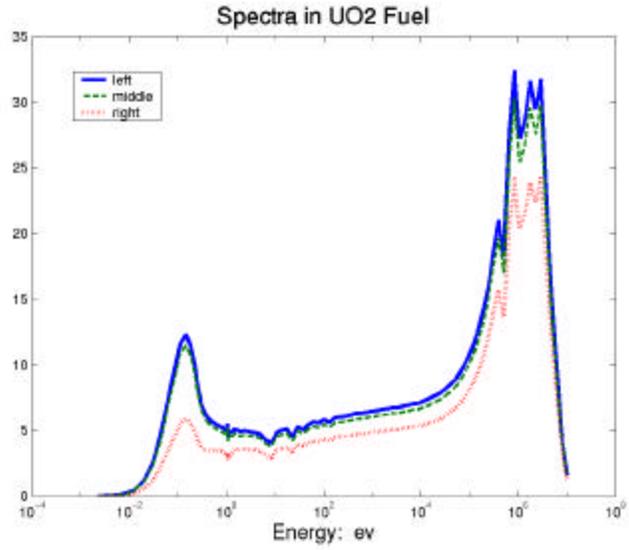


Figure 4 Neutron Spectra in UO2 Assembly

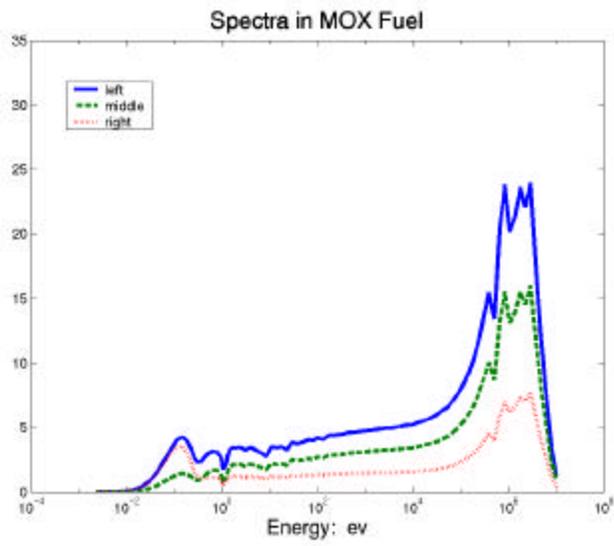


Figure 5 Neutron Spectra in MOX Assembly

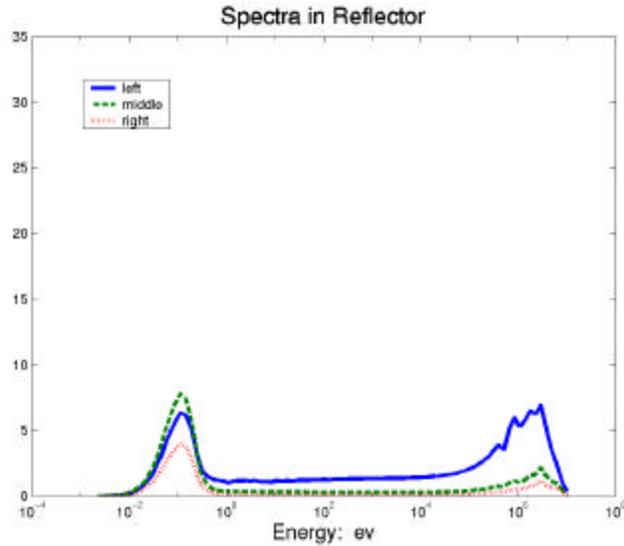


Figure 6 Neutron Spectra in the Reflector

Several remedies have been proposed and have been incorporated into some of the production codes used in the nuclear industry. These methods generally involve some type of "rehomogenization" which adjusts the few group constants based on the ambient core conditions [Rahnema, 1990], [Smith, 1994], [Chao, 1998]. Palmtag [Palmtag, 1997] recently analyzed the two group constants in a one-dimensional UO<sub>2</sub>-MOX problem with different enrichments. He observed that the effect of the spectrum change must be presented in two terms, the fast neutron leakage and spectrum interaction, and cast these two factors into leakage and spectral correlations, respectively, which have been incorporated in the nodal code SIMULATE-3K [Smith, 1997], [Palmtag, 1998].

One of the most promising recent advances towards eliminating or significantly reducing homogenization errors is the work of Lewis et al. [Lewis, 1998] in the development of "subelement" nodal methods which explicitly represent detailed pin cell geometry during the whole core transport calculations. The authors implemented their method in the ANL variational nodal code VARIANT [Palmiotti, 1995] and performed 7-group calculations on the C5 MOX Benchmark problem [Smith, 2000]. The authors compared their solutions with and without pin cell homogenization and noted significant reductions in the error of both the eigenvalue and pin power distribution.

### *The Spatial Discretization Effect*

The original coarse mesh nodal methods relied upon fourth order polynomials to describe the flux shape within a node [Finnemann, 1977], [Lawrence, 1986]. Several researchers [Joo, 1997] have shown that polynomials can not adequately describe the severe flux gradients between uranium and mixed oxide fuel assemblies. This can be demonstrated using the MOX benchmark problem. As shown in Figure 7, the quartic polynomial solution for the thermal group flux shown as "NEM" differs substantially from the analytic solution shown as "ANM". The "exact" thermal flux for this problem was shown in Figure 3.

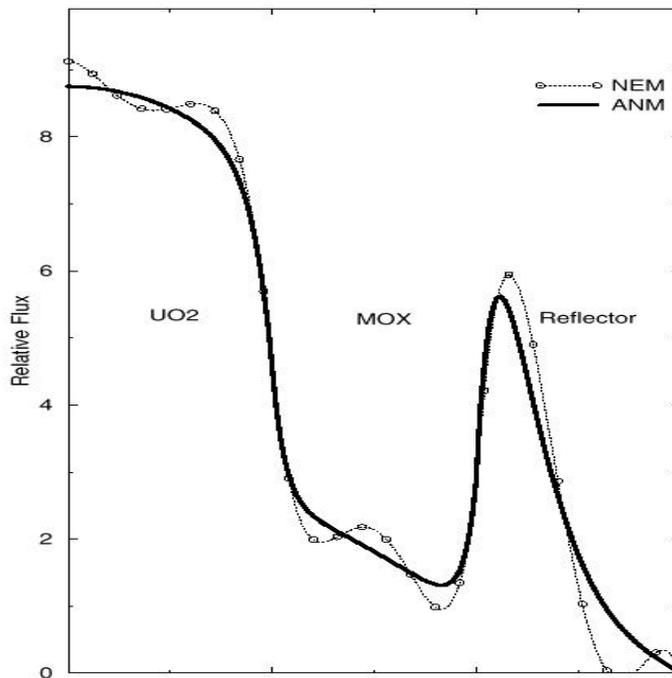


Figure 7 Thermal Flux Comparison in the 1D MOX Benchmark

A particular concern with the NEM solution is that it predicts non-physical fluctuation in the fuel region and negative fluxes in the core reflector region. This can lead to substantial errors in the fuel power predictions and significant numerical problems with the solution algorithms. Several "hybrid" ANM methods have been developed in last decade [Esser, 1993], [Joo, 1997] that incorporate hyperbolic functions in the basis of the flux expansion and accurately predict the node flux variation of MOX fueled nodes.

Modifications to spatial discretization methods were also required for the flux reconstruction or “dehomogenization” methods used to predict the pin powers in the advanced nodal codes. These modifications include the use of explicit two group “form functions” to incorporate the intra-assembly flux distribution [Shatilla, 1997]. Comparisons to Monte Carlo and MOX benchmark problems [Caverac, 1994], [Lefevbre, 1991] indicate that the pin-wise fission rates for MOX fueled cores can be predicted to within 1% of fine mesh reference results using the nodal flux solution and pin power reconstruction [Smith, 1997].

### *The Group Collapsing Effect*

Current light water reactor calculations utilize two energy groups for the global core calculation. This has proven adequate for cores fueled with uranium dioxide fuel. However, the presence of significant amounts of plutonium in the core creates a hardened neutron spectrum in which the neutron interaction and transport effects in the epithermal region can be significant. There is evidence [Taiwo, 1998] that more than two energy groups may be necessary to adequately capture the important physics effects. The eigenvalue error from performing the MOX benchmark problem with various numbers of energy groups is shown in Table 1. As indicated, the error in the two group solution is reduced by 70% and 83% when using 4 and 8 energy groups, respectively.

Table 1 Eigenvalue Comparison with Different Numbers of Energy Groups

Number of Groups	K_eff	Error: pcm
97	1.29073	-
8	1.29109	36
4*	1.29135	62
2	1.29284	211

\*Energy group boundaries are 0.625eV, 4eV, and 0.82 MeV

The substantial reduction in the error achieved by increasing the number of groups from 2 to 4 can be understood by examining the plutonium resonances in Figure 8. The group 3 boundary was chosen to isolate the large Pu resonances. As indicated in Figure 9 which shows the group fluxes for the four group result, the shape of the third group flux at the interface is significantly different than the group 1 and group 2 fluxes. The neutron currents and leakages are more accurately predicted with the 4 group structure and hence the eigenvalue is significantly reduced.

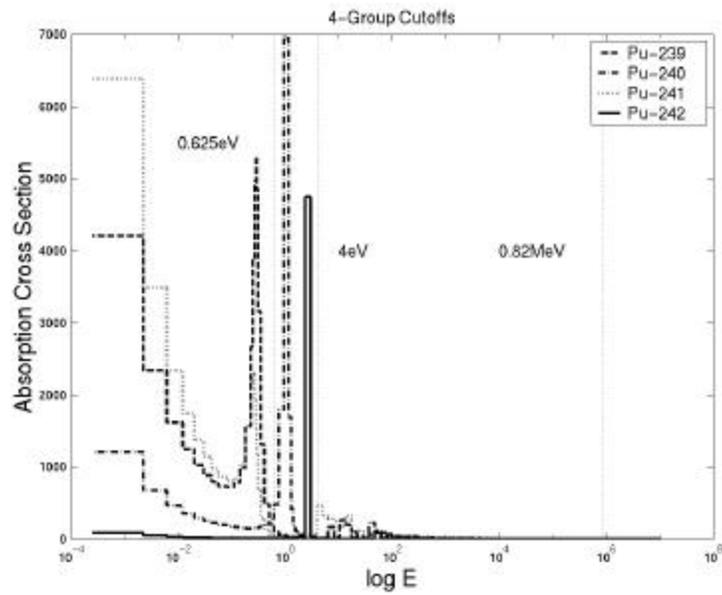


Figure 8 Pu Cross Sections and Energy Cutoffs

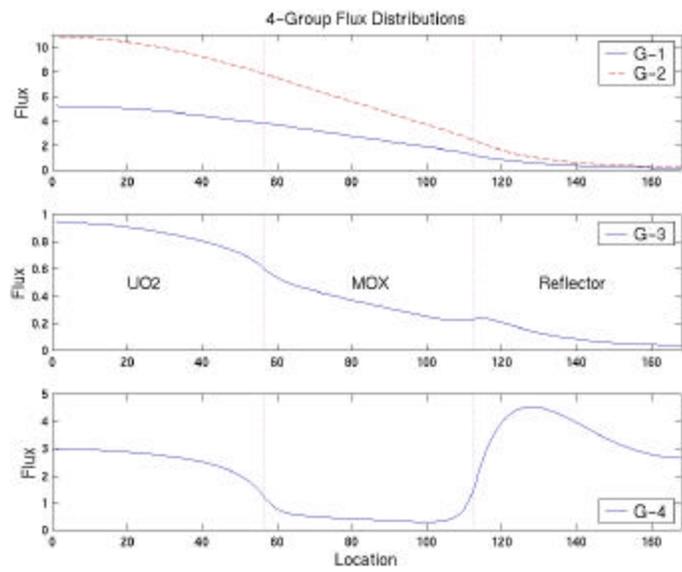


Figure 9 Four Group Fluxes for 1D MOX Benchmark Problem

### *The Transport Effect*

The severe material changes at the interface between uranium and mixed oxide assemblies can lead to significant neutron streaming effects. The presence of strong "transport effects" brings into question the validity of the P1 or diffusion approximation to the transport equation. Several researchers have suggested that higher order approximations to the transport equation such as P3 are necessary for MOX fuel problems [Brantley, 1999].

The transport error can be demonstrated using the MOX benchmark problem. The difference in the eigenvalue of the 97 group diffusion (P1) solution and the exact reference is 177 pcm. A 97 group P3 calculation was then performed and the error was reduced to 54 pcm. The error in the power distribution of the P1 and P3 solutions relative to the reference is shown in Figure 8 for the UO<sub>2</sub>/MOX interface where the highest power fuel pin occurs. As shown in the Figure, the maximum error in the P1 solution is reduced by about 50%, which is consistent with the results of other researchers [Mengelle, 1999].

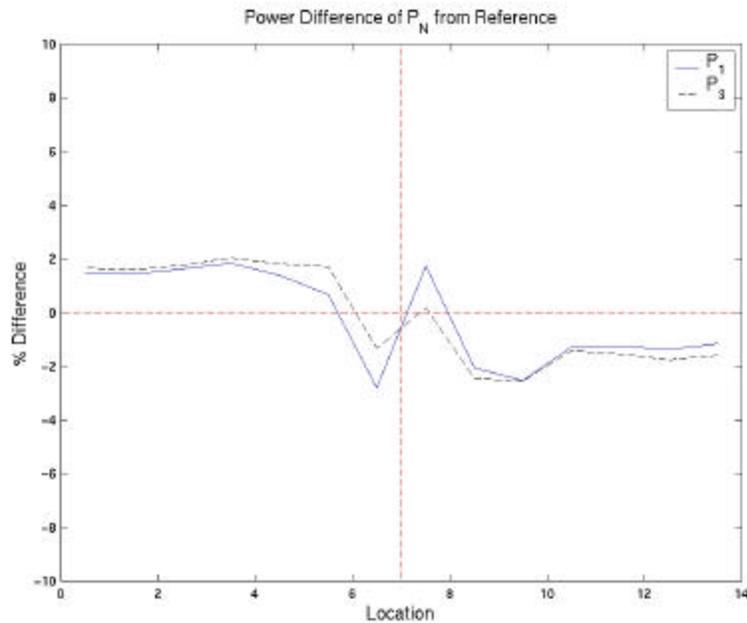


Figure 10 Pin Power Error Distribution in UO<sub>2</sub>/MOX/REF Benchmark Problem

## Summary and Conclusions

There has been concern during the last several years that the advanced nodal methods that have been developed for uranium fueled LWRs do not provide the same accuracy when applied to the same cores fueled with mixed oxide. Several modifications to the existing methods have been proposed and some have been implemented in utility and vendor codes. The purpose of this paper was to provide a framework for understanding some of the limitations in modern nodal methods and for examining some of the modifications available for improving the accuracy of MOX fuel analysis.

While modifications to the current generation of modern nodal methods have recovered much of the accuracy lost by the presence of MOX fuel, further benchmark analysis and assessment will help identify any remaining issues that must be resolved. Specifically, the work here addressed primarily steady-state neutronics, whereas additional considerations may be required for transient neutronics analysis of MOX fueled cores. Such an exhaustive benchmark and assessment effort for both steady-state and transient analysis will help reduce any perception of risk associated with weapons grade plutonium disposition in commercial Light Water Reactors.

## Acknowledgements

The authors are grateful for the support of Farouk Eltawila and the NRC Staff during the course of this work. The authors would also like to acknowledge the valuable discussions with Dave Diamond from Brookhaven National Laboratory.

## References

- [Brantley, 1998] P. Brantley, D. I. Tomasevic, and E. W. Larsen, "Application of the Simplified PN Approximation to Mixed-Oxide Fuel Problems," Transactions of the American Nuclear Society, vol. 79, pp. 173-4, (1998).
- [Cavarec, 1994] C. Cavarec, J. F. Perron, D. Verwaerde, J. P. West, "Benchmark Calculations of Power Distribution within Assemblies," HT-12/94006 A, NEA/NSC/DOC (94) 28, EDF 1994.
- [Chao, 1998] Y.A. Chao, Y. A. Shatilla, T. Ida, Y. Tahara, "Challenges to Nodal Diffusion Methods for Cores with Mixed Oxide Fuel", *Proc. International Conference on the Physics of Nuclear Science and Technology*, Long Island, NY, Oct., 1998, pp 9-14.
- [Edenius, 1991] M. Edenius, CASMO-4 Documentation, Studsvik, 1991.
- [Edenius, 1998] M. Edenius, D. Knott, K. Smith, "CASMO-SIMULATE on MOX Fuel," *Proceedings International Conference on the Physics of Nuclear Science and Technology*, Long Island, NY, October 5-8, 1998, pp. 135-142.
- [Esser, 1993] P. D. Esser, K. S. Smith, "A Semianalytic Two-Group Nodal Model for SIMULATE-3," Transactions of American Nuclear Society, San Diego, California, Vol. 68, 220-222, June, 1993.

- [Finck, 1998] P. Finck, et al., "Compared Performances of ENDF/B-VI and JEF-2.2 for MOX Core Physics," *ANS Transactions*, Vol. 79, Nov. 1998.
- [Finnemann, 1977] H. Finnemann, F. Bennowitz, M. R. Wagner, "Interface Current Techniques for Multidimensional Reactor Calculations," *Atomkernenergie*, 30, 123-128(1977).
- [Jones, 1997] D. Jones, et al., "CPM-3 Computer Code Manual," Volume 1: Theory and Numerics Manual, EPRI RP-3418, Sep., 1997.
- [Joo, 1997] H. G. Joo, G. Jiang, T. J. Downar, "A Hybrid ANM/NEM Interface Current Technique for the Nonlinear Nodal Calculation," *Proc. ANS Conf. Math. Comp.*, Saratoga, NY, Oct., 1997.
- [Joo, 1999] H. K. Joo, H. G. Jung, T. K. Kim, J. M. Noh, Y.J. Kim, "Verification of HELIOS and HELIOS/AFEN Against PWR Critical Experiments Loaded with High Plutonium Content MOX Fuels," *Annals of Nuclear Energy*, 26 (1999) 917-924.
- [Lawrence, 1986] R. Lawrence, "Progress in Nodal Methods for the Solution of the Neutron Diffusion and Transport Equations," *Nuclear Science and Engineering*, 123, 403-414 1986).
- [Lefevbre, 1991] J. Lefevbre, et al., "Benchmark Calculations of Power Distributions within Assemblies," NEACRP-L-336, October, 1991
- [Lewis, 1998] E. Lewis, G. Palmiotti, "A Finite Subelement Formulation of the Variational Nodal Method," *ANS Trans.*, **79**, 144 (1998).
- [Maldague, 1998] T. Maldague, et al., "Belgian Programmes for MOX Fuel Validation," *OECD Meeting on Physics and Performance of Reactor Based Plutonium Disposition*, Paris, France, September, 1998.
- [Mengelle, 1999] S. Mengelle, et al., "A New Power Reactor 3D Transport Calculation Scheme Using the CRONOS2 and APOLLO2 Codes," *PHYSOR-2000*, Madrid, Sep., 1999, pp. 1047-1054.
- [Palmiotti, 1995] G. Palmiotti, E. Lewis, C. Carrico, "VARIANT: VARIational Anisotropic Nodal Transport for Multidimensional Cartesian and Hexagonal Geometry Calculation, Argonne National Laboratory, ANL-95/40, 1995.
- [Palmtag, 1997] Scott Palmtag, "Advanced Nodal Methods for MOX Fuel Analysis", Ph.D thesis, MIT, Aug. 1997
- [Palmtag, 1998] Scott Palmtag, K. S. Smith, "Two-Group Spectral corrections for MOX Calculations", *Proc. International Conference on the Physics of Nuclear Science and Technology*, Long Island, NY, Oct., 1998.
- [Rahnema, 1990] F. Rahnema, "Influence of Flux gradients on Local and Global Reactivities in BWRs", *Proc. Int. Conf. Physics of Reactors: Operation, Design and Computation*, Marseille, France, April 23-27, 1990.
- [Savelli, 1998] P. Savelli, *OECD Meeting on Physics and Performance of Reactor Based Plutonium Disposition*, September, 1998, Paris, France.
- [Shatilla, 1997] Y. Shatilla, "Westinghouse Advanced Nodal Code with Pin-power Reconstruction for MOX Applications," *ANS Transactions*, Orlando, FL., Vol. 76, 179, June, 1997.
- [Smith, 1994] K. S. Smith, "Practical and Efficient Iterative Method for LWR Fuel Assembly Homogenization", *ANS transaction*, Vol. 71, 238-241(1994).
- [Smith, 1997] K. Smith, "MOX Analysis Methods for SIMULATE-03," *ANS Transactions*, Orlando, FL., Vol. 76, 181, June, 1997.
- [Smith, 2000] M. Smith, N. Tsoufanidis, E. Lewis, G. Palmiotti, T. Taiwo, "Whole-Core Neutron Transport Calculations Without Cross Section Homogenization," *ICONE-8*, April, 2000.
- [Taiwo, 1998] T. Taiwo, et al., "Development of Three-dimensional Transport Analysis Capability for LWR MOX Analysis," *ANS transactions*, Vol. 79, Nov., 1998