

# OPTIMIZATION OF MOX ENRICHMENT DISTRIBUTIONS IN TYPICAL LWR ASSEMBLIES USING A SIMPLEX METHOD-BASED ALGORITHM

**G. F. Cuevas Vivas**

*Gerencia de Energía Nuclear  
Instituto de Investigaciones Eléctricas  
Av. Reforma 113, Col. Palmira  
62490 Temixco, Morelos (México)*  
[gfcuevas@iie.org.mx](mailto:gfcuevas@iie.org.mx)

**T. A. Parish, G. L. Curry**

*Nuclear Engineering Department and Industrial Engineering Department  
Texas A&M University  
College Station, Texas (U. S. A.) 77843-3133*  
[tap@trinity.tamu.edu](mailto:tap@trinity.tamu.edu), [g-curry@tamu.edu](mailto:g-curry@tamu.edu)

## ABSTRACT

The enrichment distributions within Light Water Reactor (LWR) fuel assemblies are optimized using a modified linear programming (SIMPLEX Method) technique initiated from a flat enrichment distribution until a target, maximum local power peaking factor is achieved. The optimum rod enrichment distribution when each rod is allowed to have its own individual enrichment (for this case the target, maximum local power peaking factor is 1.0) is obtained at an intermediate point of the optimization procedure. Later, the optimal locations and values for a reduced number of rod enrichments (groups) are obtained for an input target maximum local power peaking factor by applying sensitivity to change techniques. After an initial set of enrichment groups have been defined, interchanges of rods among neighboring groups are carried out to obtain the final assembly enrichment distribution. The optimization procedure is demonstrated by presenting results for both Boiling Water Reactor (BWR) and Pressurized Water Reactor (PWR) fuel assembly designs. Reactor-grade plutonium (with a fissile Pu fraction of 59.6%) and weapons-grade plutonium (with a fissile Pu fraction of 94.0%) were assumed to be the feed Pu material for the MOX fuel rods in the BWR and PWR examples, respectively. Hot-full-power-temperature and beginning-of-life conditions were also assumed in the example problems.

# 1. INTRODUCTION

The detailed design of a fuel assembly is not so large a problem that current computer resources limit the designer from obtaining relatively complete derivative information. With the use of an accurate nuclear model, the obtained derivative information can be employed not only to find the optimal rod enrichments<sup>1</sup> for the case when the maximum local power peaking factor is 1.0 (each rod is allowed to have a different enrichment) but also to rank the rod positions according to their effect on the maximum local peaking factor and thereby to determine optimal enrichment distributions for target maximum local power peaking factor values that are greater than 1.0. Given that the number of variables is modest, the feasibility and quality of candidate configurations can be evaluated accurately using state-of-the-art reactor physics programs that guide the search without requiring excessive computer resources. This study describes a SIMPLEX algorithm<sup>2</sup> that has been applied along with the WIMS7b program to determine optimal assembly enrichment distributions for typical LWR assemblies containing either fresh Low Enriched Uranium (LEU) and plutonium Mixed Oxide (MOX) fuels. MOX isotopics for both reactor-grade and weapons-grade plutonium were utilized to demonstrate the wide-range of applicability of the optimization technique.

This paper presents a method that makes more extensive use of derivative information than in many previous studies<sup>1</sup>. Sensitivity information regarding the effects of enrichment at each rod position on the maximum local peaking factor inside the assembly are used to obtain the final enrichment distribution. The positions and numbers of fuel rods (using a minimum number of different MOX enrichments) are calculated so as to achieve a user-specified value for the maximum local power peaking factor in the assembly. The optimization methodology is flexible enough to allow the calculation of MOX enrichment distributions under a variety of “neutronic” heterogeneities such as the presence of gadolinium rods, internal moderator regions, or neighboring LEU fuel assemblies. In the example problems, layouts, materials and dimensions were used that resemble the configurations of modern assemblies utilized in commercial Boiling Water Reactors (BWRs) and Pressurized Water Reactors (PWRs). The use of fresh fuel was intentionally chosen in order to set limits on the problem and facilitate the discernment of the rod position-enrichment relationships. Also, the tendency to yield high local power peaking factors is expected when fresh fuel is present assuming ordinary fuel assembly designs and conditions. The final contribution of this study is to present a full deterministic technique capable of providing assembly enrichment distributions (using small numbers of enrichment groups) such that a maximum local power peaking factor criterion is met.

In the optimization examples presented here, the within assembly, rod power distributions and the rod position-enrichment sensitivities were obtained using WIMS7b<sup>3</sup>. The WIMS7b model used a sixty-nine energy group nuclear data library derived from the latest JEF 2.2 library and the CACTUS two-dimensional transport module.

## 2. FUEL ASSEMBLY MODELS

Two fuel assembly models were selected to illustrate the optimization methodology. The first model corresponded to a BWR fuel assembly type known<sup>4</sup> as ATRIUM<sup>TM</sup>-10. It consists of a  $10 \times 10$  array of fuel rods, a central water channel that occupies the space of nine fuel rods, and employs six fuel rods that contain gadolinium. For the optimization example problem, the assumed assembly average enrichment was 4.17 w/o of Pu fissile. Reactor-grade plutonium was used in the MOX fuel rods. The gadolinium rods (with a  $Gd_2O_3$  content of 1.5 w/o) were fueled by U-235 with a constant enrichment of 3.95 w/o. Material and geometry data for the optimization analysis were taken from the specifications for a recently proposed benchmark problem<sup>5</sup>.

The second optimization example was based on using MOX in PWRs. It employed a WIMS7b model based on a colorset formed by the quadrants of four neighboring  $17 \times 17$  Westinghouse PWR type assemblies. MOX assemblies were located in the northeast (NE) and southwest (SW) corners, respectively. The other assemblies were fuelled with LEU. The isotopics for the MOX fuel corresponded to that of weapons-grade plutonium (fissile Pu fraction of 94.0%) and the assembly average Pu-fissile content was taken to be 4.872 w/o. All of the rods in the LEU assemblies were assumed to have a U-235 enrichment of 4.1 %. A boron concentration of 500 ppm was assumed in the water (moderator). There were 24 Wet Annular Burnable Absorber (WABA) rods and 1 instrument tube in the MOX assembly, and 25 guide thimbles in the LEU assemblies<sup>6-7</sup>.

## 3. OPTIMIZATION METHODOLOGY

The optimization methodology can be summarized with the following seven steps:

1. The relative rod power is computed with a single-valued enrichment distribution.
2. Power sensitivity coefficients of first order are computed with a series of rod power evaluations using an assembly analysis code for individual rod enrichment changes. The sensitivity matrix is computed and stored.
3. The linear programming algorithm is employed to find an improved enrichment distribution based on the sensitivity coefficients calculated in the previous step. The algorithm computes a vector whose components are estimated rod material perturbations (relative rod enrichments) to flatten the relative power distribution based on the sensitivity matrix and the problem constraints. An imposed constraint is that the average assembly enrichment remains constant.
4. The estimated relative rod enrichments to obtain a flat power distribution are used in WIMS7b to see if the obtained distribution is flat. If not, updated values for the sensitivity

coefficients are computed using WIMS7b to evaluate the effect of a single rod's enrichment as in step 2. Then step 3 is repeated. Steps 2 and 3 are repeated until an optimum relative power distribution (maximum local power peaking factor of 1.00) is obtained. To obtain this optimum relative power distribution each rod is allowed to have its own value of enrichment. The corresponding rod enrichments are referred as the vector of optimum rod enrichments. In this case, the number of allowed enrichments equals the number of different rods within the assembly after accounting for symmetry. This optimized enrichment distribution is referred as the flat-power-distribution (FPD) enrichment distribution.

5. The sensitivity matrix stored from an earlier stage of the iterative process is used to construct a first-order model for predicting "new" relative rod power distributions. This model is used to estimate the maximum allowed enrichment increase in each rod to obtain a specified maximum local power peaking factor assuming that the rest of the rods are maintained at their optimum enrichment. The optimum rod enrichments are ordered, from lowest to highest. This ordering links rod position with optimum rod enrichment. The sorting is used to "group" locations to be assigned the same enrichment. Based on a target maximum local power peaking factor, the sensitivity matrix is inverted to estimate the maximum local power peaking factor as the enrichments are modified from the FPD values. After the enrichment changes to achieve the target maximum local power peaking factor have been estimated by this procedure, a full WIMS7b calculation is performed to verify the accuracy of the modified enrichment distribution.
6. The rod enrichment grouping starts with the two lowest optimum rod enrichments first and it proceeds by averaging together the individual enrichments to obtain the enrichment value corresponding to group "1". The grouping process proceeds adding one enrichment at a time and calculating the group enrichment value by averaging together the enrichments that belong to the created group "g". Then, the rod enrichment grouping uses the first-order model and the target value for the maximum local power peaking factor to define how many rod enrichments will belong to the group "g". If the maximum local power peaking factor (computed with the first-order model) exceeds the target value for the maximum local power peaking factor, the last grouped optimum rod enrichment is retired from the group "g", the group "g" is closed, and a new group, "g+1", is initiated. The grouping finishes when the highest optimum rod enrichment has been included into an enrichment group.
7. After the enrichment groups have been defined, interchanges of rods among neighboring groups are carried out. The enrichment distributions are evaluated using WIMS7b. The final "grouped" enrichment distribution that meets the target maximum local power peaking factor is output.

The two major parts of the methodology, namely the computation of the optimum relative rod power distribution and rod enrichment grouping, will be described in the following sections.

### 3.1. COMPUTATION OF THE OPTIMUM RELATIVE ROD POWER DISTRIBUTION

An optimum relative rod power distribution (maximum local power peaking factor of 1.00) for a typical LWR type assembly will be calculated by using the rod fission rates and keeping the assembly average enrichment constant to satisfy reactivity requirements. The methodology is based on the following four elements:

1. An altered fission rate distribution (denoted by  $F'$ ) is constructed from the function that describes the assembly fission rate (denoted by  $F$ ). Each component of the altered fission rate distribution is the rod fission rate multiplied by a positive amount that alters the rod fissile content and therefore, the rod power. Each rod factor is referred as perturbation factor (denoted as  $\lambda'_j$  for the rod  $j$ ). Only the set of perturbation factors that reduced the maximum power peaking factor of the assembly fission rate ( $F$ ) is accepted by the optimization methodology. Then, each perturbation factor is incorporated to the rod enrichment, the methodology searches for a new set of perturbation factors and the process repeats again until the maximum local power peaking factor is equal to 1.00. Once the optimization strategy obtains convergence, the functions  $F$  and  $F'$  will be identical, each perturbation factor will be equal to 1 and the optimum set of enrichment factors will have as many elements as different rod types were defined in the assembly model.
2. The accurate evaluation of the fission rate in each rod is of primal importance because knowing the sensitivity to small fissile material changes will be required for the optimization process. Additionally, the presence of neutron flux perturbing elements, such as, absorption elements and water holes, will increase the nonlinearity of the assembly fission rate. Therefore, a reliable, accurate code is needed to solve the neutron transport equation to determine the fission rate and its sensitivity to material changes. Each re-evaluation of the fission rate distribution can be conceptualized in terms of the optimization strategy as an updating of the “cost” coefficients of the objective function.
3. Each rod’s enrichment will be described relative to the assembly average enrichment,  $\bar{N}$ , and by using a factor  $\lambda \equiv N_j / \bar{N}$ , where  $N_j$  is the enrichment of rod “ $j$ ”. The vector containing the enrichment factors for all the rods will be called the enrichment factor vector. The total number of rod enrichments will be denoted by  $M$ , that is also the number of different rods in the assembly model after accounting for symmetry.
4. Both, the enrichment and the perturbation factors, denoted by  $\lambda_j$  and  $\lambda'_j$  for each rod  $j$ , respectively, are positive and have an average value of one. They are forced to satisfy a normalization condition that ensures the assembly average enrichment is a constant. From the point of view of the optimization methodology, these factors are conceptualized differently. The enrichment factors,  $\lambda_j$ , are viewed as the “accepted” or current fissile content for the rod  $j$ , whereas the perturbation factors,  $\lambda'_j$ , are considered to be the “candidate” alteration of the rod fissile material to flatten the relative power distribution. Once the set of perturbation factors is accepted by the optimization methodology, the enrichment factors are updated by the inclusion of the former perturbation factors and the process repeats. At the beginning of

the optimization process, all of the enrichment factors are equal to one. This condition is named Flat Enrichment Distribution (FED). On the other hand, when the maximum power peaking factor is equal to 1.00 (optimization process has converged) all of the perturbation factors are equal to one and the optimization process stops.

In the present study, most of the assembly design parameters, such as, rod and clad materials, rod pitch and configuration of flux perturbing elements, will be adopted from values for typical LWR assembly designs. Only the rod enrichments will be the variables utilized to optimize the relative rod power distribution.

### 3.2. ROD ENRICHMENT GROUPING

The fission rate distribution was flattened at each optimization stage by updating the cost vector until an optimum set of material alteration factors was obtained  $\{\lambda_j^*\}_{j=1}^M$ . However, due to economic constraints on the assembly manufacturing process, it is not feasible to employ the full  $M$  number of enrichments in commercial nuclear fuel assemblies. Therefore, a reduction of this number is considered in order to obtain a realistic assembly design. For this purpose, the derivative (sensitivity) information was utilized in a linear model to predict the increment to the relative rod powers when the rod enrichments are modified from their FPD values and to ensure that the maximum local power peaking factor does not exceed a target value. The individual rod enrichments are replaced with an average enrichment value (group enrichment) that is calculated by combining rods to form groups. The rod grouping process is done by evaluating the inclusion of one rod at the time into a particular group, and in a sequenced manner described as follows,

- 1) A limiting maximum local power peaking factor,  $P_{\max}$ , is specified as the target for the new “grouped” enrichment distribution. This input parameter is the only user-specified value,
- 2) The rods are ranked according to the value of their optimum enrichment factor,  $\lambda^*$ ; and a ranking number is assigned to each rod. The grouping process starts by including the two rods with the lowest  $\lambda^*$  values to begin formation of the first group,
- 3) A new enrichment factor ( $\lambda^g$ ) for the group is calculated from the arithmetic average of the  $\lambda^*$  values for the rods that belong to a group,
- 4) The model employs a set of linear equations, represented by the matrix  $A$ , to estimate the change in the relative rod powers as a function of the change of the rod’s enrichment to the group value. For example, when rod  $j$  is tested to become a member of the rod group  $g$ , its relative power,  $P_{j,\text{new}}$ , must not exceed the predetermined target maximum local power peaking factor ( $P_{\max}$ ) according to the equation,

$$P_{j,new} = 1.0 + \frac{1}{\lambda_j^*} A_j^{-1} (\lambda^g - \lambda^*) \leq P_{\max} \quad (1)$$

where  $\lambda^g$  and  $\lambda^*$  are the vectors for the group and optimum enrichment factors, respectively, and  $A_j^{-1}$  is the row of matrix  $A^{-1}$  that corresponds to the rod enrichment  $j$ .

- 5) If equation (1) is satisfied, the grouping process takes the next ranked rod and evaluates its inclusion into the group; otherwise, the current group is closed and a new group,  $g + 1$ , is started,
- 6) The rod grouping process is finished when the last rod is included in the last group,
- 7) Finally, testing of slightly modified configurations is performed. That is, the rods that are the last and the first in neighboring groups are interchanged between the neighboring groups. The changes in the maximum local power peaking factor are then evaluated with the assembly analysis code WIMS7b and if the peak value is lowered, the new shuffled configuration is accepted. The number of modified configurations is about twice the number of new groups. The advantage of this analysis is that it ensures that the final configuration is close to the best possible one.

#### 4. MATHEMATICAL STATEMENT OF THE OPTIMIZATION PROBLEM

Consider that the total fission rate of the assembly is given by the function  $F$  that is defined as

$$F = \sum_{j=1}^M f_j = V \sum_{j=1}^M N_j \sigma_j \phi_j \quad (\text{fissions/s}) \quad (2)$$

where

- $M$  = total number of rods in the assembly,
- $f_j$  = rod fission rate,
- $N_j$  = rod enrichment (fissile atoms/cm<sup>3</sup>),
- $\sigma_j$  = microscopic fission cross section (cm<sup>2</sup>),
- $\phi_j$  = scalar neutron flux (neutrons/cm<sup>2</sup> s),
- $V$  = fuel rod volume (cm<sup>3</sup>).

The function  $\sigma_j \phi_j$  (neutrons/s) is non-linear and depends strongly on rod enrichment and moderation conditions in the neighborhood of the rod. An accurate evaluation of this function for each rod is of extreme importance for a detailed description of the nuclear behavior of the assembly. The function  $\sigma_j \phi_j$  and each enrichment factor can be expressed in terms of their

assembly average values and a deviation,

$$\begin{aligned}\lambda_j &= 1 + \Delta\lambda_j \\ \sigma_j\phi_j &= \overline{\sigma\phi} + \Delta(\sigma\phi)_j\end{aligned}\quad (3)$$

The assembly total fission rate can be as,

$$\begin{aligned}F &= \overline{NV} \sum_{j=1}^M \lambda_j \sigma_j \phi_j = \overline{NV} \sum_{j=1}^M [1 + \Delta\lambda_j][\overline{\sigma\phi} + \Delta(\sigma\phi)_j] \\ &= M \overline{N \sigma\phi} V + \overline{NV} \sum_{j=1}^M \Delta(\sigma\phi)_j \Delta\lambda_j \\ &= F_o + \overline{NV} \sum_{j=1}^M \Delta(\sigma\phi)_j \Delta\lambda_j\end{aligned}\quad (4)$$

#### 4.1 ALTERED ASSEMBLY FISSION RATE

The consideration of a material perturbation in each rod by a new (positive) factor  $\lambda'_j$  will define an altered assembly fission rate distribution,  $F'$

$$\begin{aligned}F' &\equiv V \sum_{j=1}^M N_j \sigma_j \phi_j \lambda'_j = \overline{NV} \sum_{j=1}^M \lambda_j \sigma_j \phi_j \lambda'_j \\ F' &\equiv \sum_{j=1}^M f_j \lambda'_j\end{aligned}\quad (5)$$

In terms of average values, the last expression can be re-written as

$$F' = \overline{NV} \sum_{j=1}^M [1 + \Delta\lambda_j][\overline{\sigma\phi} + \Delta(\sigma\phi)_j][1 + \Delta\lambda'_j] \quad (6)$$

After some manipulation,

$$F' = \underbrace{M \overline{N \sigma\phi} V + \overline{NV} \sum_{j=1}^M \Delta(\sigma\phi)_j \Delta\lambda_j}_F + \underbrace{\overline{N \sigma\phi} V \sum_{j=1}^M \Delta\lambda_j \Delta\lambda'_j}_{P_i}$$



$$+ V \underbrace{\sum_{j=1}^M N_j \Delta(\sigma\phi)_j \Delta\lambda'_j}_{P_{II}} \quad (7)$$

The third term,  $P_I$ , accounts for the combined effect of the increment in the enrichment and perturbation factors,  $\Delta\lambda_j$  and  $\Delta\lambda'_j$ , respectively. The fourth term in equation 7, denoted as  $P_{II}$ , has an important significance for this analysis because it will be used to define the objective function for the linear programming problem.

#### 4.2 THE OBJECTIVE FUNCTION

The value of  $\Delta(\sigma\phi)_j$  inside the  $P_{II}$ -function will be approximated using its relative change due to changes in rod enrichment. The function  $P_{II}$  can be re-written as

$$P_{II} \equiv V \sum_{j=1}^M N_j \frac{\Delta(\sigma\phi)_j}{\Delta\lambda_j} \Delta\lambda_j \Delta\lambda'_j \quad (8)$$

The ratio can be approximated by

$$\frac{\Delta(\sigma\phi)_j}{\Delta\lambda_j} \cong \sigma_j \frac{\Delta\phi_j}{\Delta\lambda_j} + \phi_j \frac{\Delta\sigma_j}{\Delta\lambda_j} \quad (9)$$

It is expected that a change in rod enrichment have a greater impact on the neutron scalar flux than on the microscopic cross section.

$$\frac{\Delta\sigma_j}{\Delta\lambda_j} \ll \frac{\Delta\phi_j}{\Delta\lambda_j} \quad (10)$$

Then, the function  $P_{II}$  is approximated to

$$P_{II} \cong V \sum_{j=1}^M N_j \sigma_j \frac{\Delta \phi_j}{\Delta \lambda_j} \Delta \lambda_j \Delta \lambda'_j \quad (11)$$

and it also can be written as,

$$\begin{aligned} P_{II} &= V \sum_{j=1}^M N_j \sigma_j \Delta \phi_j(\Delta \lambda'_j) = \\ &= V \sum_{j=1}^M N_j \sigma_j \phi_j(\Delta \lambda'_j) - V \sum_{j=1}^M N_j \sigma_j \bar{\phi}(\Delta \lambda'_j) \end{aligned} \quad (12)$$

The objective function will be defined as

$$\begin{aligned} z &\equiv P_{II} + V \sum_{j=1}^M N_j \sigma_j \bar{\phi}(\Delta \lambda'_j) = V \sum_{j=1}^M N_j \sigma_j \phi_j(\Delta \lambda'_j) \\ &= \sum_{j=1}^M f_j \Delta \lambda'_j = \sum_{j=1}^M f_j \lambda'_j - F \end{aligned} \quad (13)$$

or simply,  $z = F' - F$ .

#### 4.3 ITERATIVE SCHEME

The optimal enrichment factors are constructed at each iteration by incorporating the past perturbation factors. That is, each enrichment factor  $\lambda_j$  will be expressed as a product of previous perturbation factors  $\lambda'_j$ . The actual (calculated in the  $(k-1)$ -th iteration) enrichment factor will be given by the relation,

$$\lambda_j^{(k-1)} = \prod_{i=1}^{k-1} \lambda_j^{(i)} = \lambda_j^{(k-1)} \lambda_j^{(k-2)} \quad (14)$$

where the super-index in parenthesis indicates the iteration number. The updated rod enrichment is,

$$N_j^{(k)} = \lambda_j^{(k-1)} \bar{N} \quad (15)$$

The general relation for the perturbed fission rate will be

$$F^{(k)} = F^{(k)} + \underbrace{\bar{N} V \bar{\sigma} \phi \sum_{j=1}^M \Delta \lambda_j^{(k-1)} \Delta \lambda'_j{}^{(k)}}_{P_I} + \underbrace{\bar{N} V \sum_{j=1}^M \lambda_j^{(k-1)} \Delta (\sigma \phi)_j^{(k)} \Delta \lambda'_j{}^{(k)}}_{P_{II}} \quad (7')$$

At each optimization stage the linear objective function is,

$$z^{(k)} = \sum_{j=1}^M Cost_j^{(k)} \lambda_j^{(k)} - F^{(k)} \quad (16)$$

where the “Cost” components are the individual rod fission rates that are calculated at each stage,

$$Cost_j^{(k)} = \bar{N} \lambda_j^{(k-1)} \sigma_j^{(k)} \phi_j^{(k)} = f_j^{(k)} \quad (17)$$

#### 4.4 LINEAR CONSTRAINTS

The feasible region will be defined with a set of  $2M+1$  linear constraints for the optimization problem. These constraints can be categorized and described as follows,

1. The condition of constant value for the average assembly enrichment defines one constraint for the perturbation factors. This constraint is applied to the perturbation factors,

$$\sum_{j=1}^M \lambda'_j = M \quad (18)$$

2. The sensitivity coefficients for each relative rod power were used to establish a set of  $M$  linear inequalities. The square matrix  $A$  formed with the sensitivity coefficients as entries will be denoted as the sensitivity matrix. The system of  $M$  linear inequalities is expressed in matrix form,

$$A(\lambda^{(k)} - \lambda^{(k-1)}) \leq M \lambda^{(k-1)} \quad (19)$$

Each linear equation can be divided by its corresponding  $\lambda$ -factor. The result can be interpreted as the expected increment in relative rod power needed but whose sum cannot exceed the value of  $M$  (because  $M$  must equal to the sum of all of the relative rod powers).

To define the sensitivity matrix entries, the values of the relative rod power and the change in relative power of rod  $j$  as a function of the material alteration factor  $\lambda_j$  are defined as follows:

$$P_i^{(k)}(\lambda_j^{(k-1)}) = \frac{f_i^{(k)}(\lambda_j^{(k-1)})}{F^{(k)}/M} \quad (20)$$

$$\Delta P_{i,j}^{(k)} = \frac{f_i^{(k)}(\alpha_1 \lambda_j^{(k-1)}) - f_i^{(k)}(\alpha_2 \lambda_j^{(k-1)})}{F^{(k)}/M} \quad (21)$$

where  $\alpha_1 = 1.02$ ,  $\alpha_2 = 0.98$  for this particular application.

Sensitivity coefficients for each rod power as a function of changes in the material composition of each of the other rods can be obtained with the following relation,

$$a_{i,j}^{(k)} = \frac{\Delta P_{i,j}^{(k)}}{\frac{\alpha_1 \lambda_j^{(k-1)} - \alpha_2 \lambda_j^{(k-1)}}{\lambda_j^{(k-1)}}} \quad (22)$$

The sensitivity coefficients are approximations to the first derivative of the relative rod power as a function of a change in the rod enrichments (or perturbation factors). Their evaluation required two calculations of the fission rate for each rod using the code WIMS7b, that is, for  $M$  different types of rods,  $2M$  solutions of the neutron transport equation are required to obtain the sensitivity coefficients for all of the rods.

3. Finally, the feasible region for the perturbation factors is further defined with upper and lower bounds for the value for each perturbation factor. The upper and lower bound are

defined using the inverse of the corresponding rod power and the inverse of the PPF, respectively. These relations for the each perturbation factors represent the final  $M$  constraints

$$\frac{1}{\text{MAX } P^{(k)}(\lambda)} \leq \lambda'_i{}^{(k)} \leq \frac{1}{P_i^{(k)}}, \quad i \in M \quad (23)$$

## 5. RESULTS

### 5.1. BWR FUEL ASSEMBLY CASE

As the first example of the methodology implemented, the results for optimization of the MOX enrichment distribution within an ATRIUM-10 assembly for a case with a void fraction of 80% is presented in Figure 1. The optimized enrichment distribution, and its corresponding relative rod power distribution are given there. The optimal enrichment distribution, based on a target maximum relative rod peaking factor of 1.20, needed five different enrichments.

Table I. Comparison of the Maximum Local Power Peaking Factors Versus Void Fraction for the Benchmark Case and the Optimized Enrichment Distributions

| Case      | Moderator Void Fraction (%) |       |       |
|-----------|-----------------------------|-------|-------|
|           | 0                           | 40    | 80    |
| Benchmark | 1.229                       | 1.220 | 1.266 |
| Optimized | 1.195                       | 1.181 | 1.191 |

For further comparison, optimized enrichment distributions were obtained also for void fractions of 0% and 40%. A comparison of the maximum local power peaking factors for these optimized cases (0%, 40% and 80% void fraction) with those calculated for the benchmark problem<sup>5</sup> (using WIMS7b code) clearly favors the optimized enrichment distributions since the number of enrichment groups required is only five instead of six<sup>5</sup>. The maximum local power peaking factors are presented in Table I. However, it is worth noting that the benchmark problem may represent a typical enrichment distribution rather than an “optimum” one. The benchmark problem specifications do not comment about this. Therefore, a strict comparison should be made with caution. The optimized distributions nevertheless showed that the methodology was capable of producing what could be considered to be “improved” distributions, i.e., ones using fewer enrichments for a specified target maximum local power peaking factor, even by industrial standards.

It is also worth noting that the range for the enrichment values in the benchmark case is narrower (from 1.6 to 6.3) than the one obtained from the optimization (from 1.4 to 9). Fig. 2 shows a comparison of the number of rods in each enrichment group for both enrichment distributions. The optimized enrichment distribution selected for making this plot was that corresponding to the 80% void fraction case since in this case the liquid water that flows in the inner water channel proved to have a greater impact on the neutron moderation of the assembly. The implications and cost of the range for the optimized enrichment values have to be analyzed from the manufacturer's standpoint. For instance, constraints related to a maximum (or minimum) allowed enrichment value in the fabrication plant, the minimum number of pellets per enrichment value, and the minimum enrichment value that is economically feasible, are among the conditions that should be included as mathematical constraints in the optimization problem to obtain the enrichment distributions to be used in "real" assemblies.

In preparing the calculation for the benchmark case, the burnup calculation for the assembly model with a moderator void fraction of 40% is required. Utilizing WIMS7b the local power peaking factor as a function of burnup was calculated and compared with that of the optimized enrichment distribution. The results are shown in Table II. The optimized enrichment distribution for this particular case provides a smoother behavior of this function.

Table II. Comparison of Local Power Peaking Factor Versus Burnup for a Case of a Moderator Void Fraction of 40%.

| Case      | Burnup (GWd/t) |       |       |       |
|-----------|----------------|-------|-------|-------|
|           | 5              | 10    | 30    | 50    |
| Benchmark | 1.236          | 1.261 | 1.252 | 1.228 |
| Optimized | 1.209          | 1.197 | 1.176 | 1.111 |

## 5.2 PWR FUEL ASSEMBLY CASE

The second example considered was for optimization of the enrichment distribution for MOX assemblies surrounded by LEU assemblies in a PWR. In Reference 6, a similar colorset is discussed with a local power peaking factor of approximately 1.1 for fresh fuel and three different rod enrichments. In order to have a better comparison to results presented in reference 6, the target for the maximum local power peaking factor was searched until three enrichment groups were achieved. This target was found to be 1.08 and the local power peaking factor calculated with WIMS7b was 1.11 (see Table III).

Fig. 3 shows the optimum relative rod powers and enrichments for the different rod positions in one of the MOX assemblies ranked according to the sensitivity of the maximum local power peaking factor to changes in enrichment. Each bar corresponds to a different rod position within the assembly and has two colors. The bottom region (dark) represents the optimum value of the relative rod enrichment for the case in which each rod is allowed to have a different enrichment, i.e., the FPD case. The light-colored part of the bar represents an estimate for the maximum relative enrichment allowed for that rod if its enrichment alone were changed until the target maximum rod peaking value is reached. Figure 3 also shows the relationship of these enrichments to the three optimal enrichment “groups” represented by the three horizontal lines. The rod positions are denoted below the bars with a pair of numbers, which can be interpreted as the row and column coordinates, starting from the center of the colorset toward the NE assembly.

Fig. 4 presents the optimized MOX enrichment distribution pictorially. Fig 5 presents the relative rod power distributions for each assembly in the colorset calculated with WIMS7b. The normalizations were carried out relative to each assembly, i.e. there is a different power factor for each assembly.

Table III. Comparison of PWR Fuel Assemblies With Optimized Enrichment Distribution in the MOX Assemblies.

| Assembly Type | Relative Assembly Power (%) | Relative Assembly Absorption Rate (%) | Maximum Local Power Peaking Factor |
|---------------|-----------------------------|---------------------------------------|------------------------------------|
| <b>MOX</b>    | 102.8                       | 111.6                                 | 1.11                               |
| <b>LEU</b>    | 97.6                        | 88.4                                  | 1.23                               |

The comparison with an approximate model of a PWR colorset shows that the optimization methodology is applicable to PWR type assemblies for the case in which the MOX fuel’s isotopic composition is that of weapons-grade plutonium. Though, the configuration and composition of the absorber rods were approximated.

## CONCLUSIONS

The present implementation of the SIMPLEX method is able to accurately calculate the individual rod enrichments to obtain a flat power distribution and to provide optimal assembly enrichment distributions employing a smaller number of different enrichments conforming to a

maximum local power peaking factor target. The results include the group enrichment values, as well as, their assigned rod locations. The optimization procedure proved to be applicable in both BWR and PWR cases corresponding to typical LWR fuel assemblies, as well as, to different Pu-vector (MOX) compositions.

The optimization of enrichment distributions for the present cases was obtained utilizing accurate computational tools. The manageable number of variables in the within-assembly design problem is credited to the success of the present methodology. The present calculations were carried out on low-end desktop workstations and the CPU time needed for several linear programming iterations (approximately 4-5 for assemblies fueled with LEU and 6-7 for assemblies fueled with MOX) is only of the order of a tens of hours. The methodology, however, can easily be improved to permit a reduction in the number of power distribution evaluations needed (without sacrificing accuracy) and reducing CPU time by half.

Even though the linear programming approach was adopted much as presented in ref. 1, the new methodology utilized extensively the derivative information that was collected with the code WIMS7b in order to group the rod enrichments according to their impact on the local power peaking factor. The number of input parameters was reduced and there were no feasibility conflicts when this linearized model of the power distribution was utilized. On the other hand, the extension to innovative and stochastic algorithms would be natural and should be done in order to provide a methodology assessment. Besides this, the determination of axial enrichment distributions and the inclusion of burnup represent logical continuations of MOX usage optimization problems.

## **ACKNOWLEDGMENTS**

AEA's (WIMS7b owner and distribution company) staff is acknowledged for their technical support in the preparation of the input parameters for the WIMS7b code. The first author also acknowledges the *Consejo Nacional de Ciencia y Tecnología* for their support during his graduate studies.



## REFERENCES

- 1 Y. HIRANO, K. HIDA, K. SAKURADA, M. YAMAMOTO, “Optimization of Fuel Rod Enrichment Distribution to Minimize Rod Power Peaking throughout Life within BWR Fuel Assembly”, Nuclear Engineering Laboratory, Toshiba Corp., *J. Nucl. Sci. Technol.* Vol. 34, No. 1, p. 5-12 (1997).
- 2 S. G. NASH, A. SOFER, *Linear and Nonlinear Programming*. McGraw-Hill, New York (1996).
- 3 “The ANSWERS Software Package WIMS: A WIMS Modular Scheme for Neutronics Calculations”, User’s guide, ANSWERS/WIMS (95) 4, AEA Technology, Harwell, United Kingdom, (1996).
- 4 K. V. WALTERS, “ATRIUM<sup>TM</sup>-10 Lattice and Fuel Assembly Design”, *ANS Proceedings of the Topical Meeting: Adv. in Nuclear Fuel Management II*, **1**, Myrtle Beach, South Carolina, 3-1, (1997).
- 5 G. SCHLOSSER, W. TIMM, “Proposal for a BWR MOX Benchmark”, NEA/NSC/DOC (98)10. Revision 1, OECD Nuclear Energy Agency, Issy-les-Moulineaux, France (1998).
- 6 A. ALSAED, “Disposition of Weapons-Grade Plutonium in Westinghouse Reactors”, ANRCP-NG-ITWD-96-14, Amarillo National Resource Center for Plutonium, Amarillo, Texas (1996).
- 7 C. NA, E. SARTORI, “Benchmark on the VENUS-2 MOX Core Measurements”, NDB/99/0371/cem, OECD Nuclear Energy Agency, Issy-les-Moulineaux, France (1999).

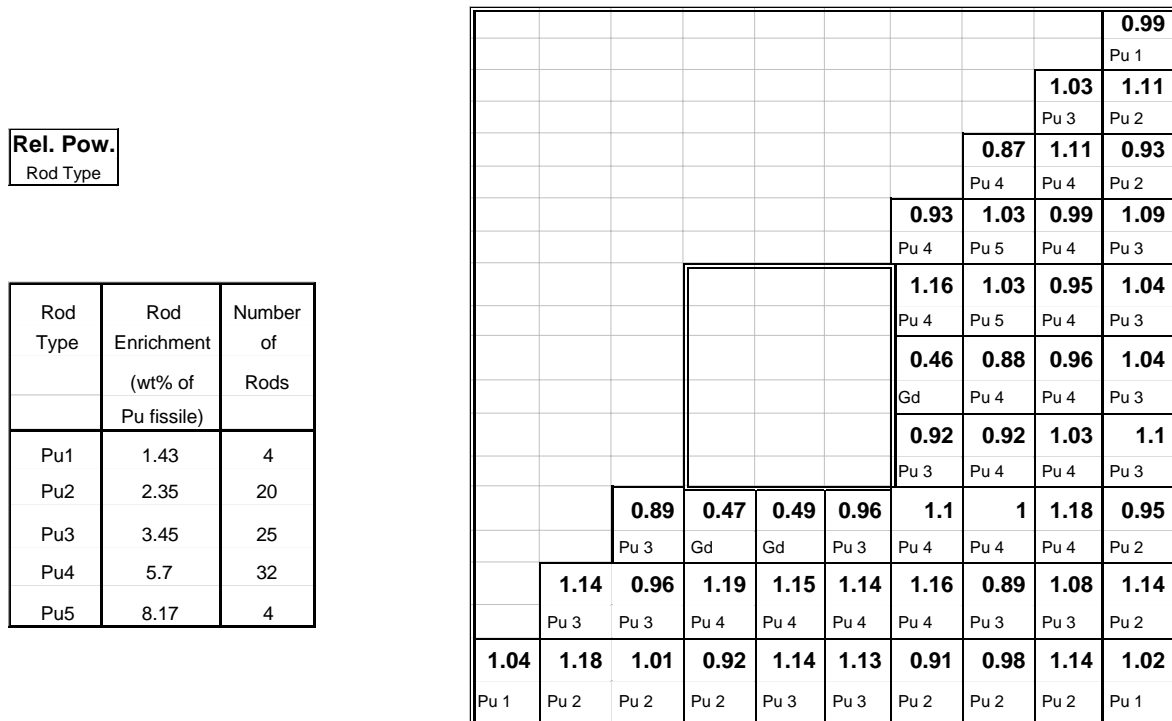


Fig. 1. Final relative rod power distribution (using five enrichments) for a target maximum local power peaking factor of 1.20 in the BWR fuel assembly.

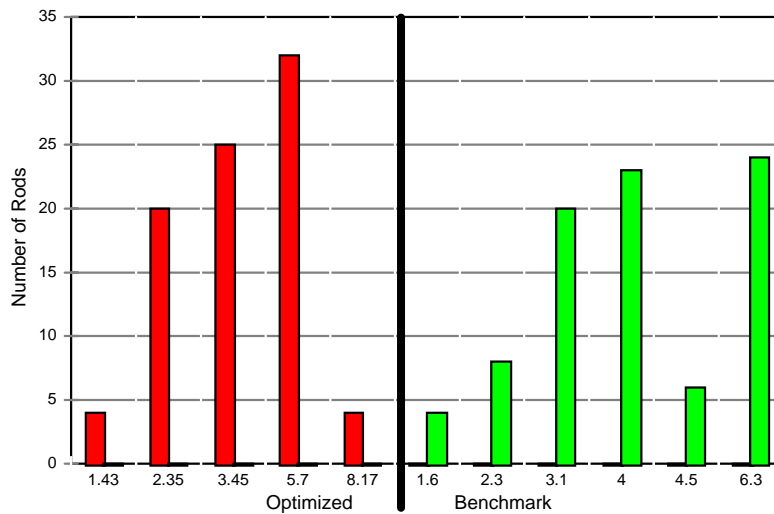


Fig. 2. Comparison of the number of rods per enrichment value for the benchmark case and for the optimized case with a moderator void fraction of 80%.

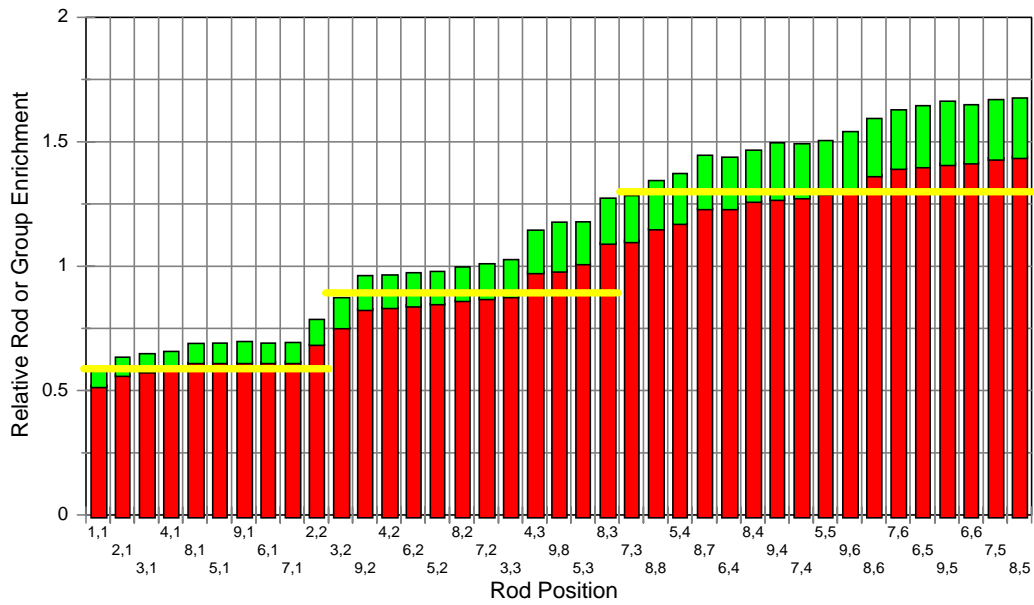


Fig. 3. Optimum enrichment factors versus rod position for PWR fuel assembly case.

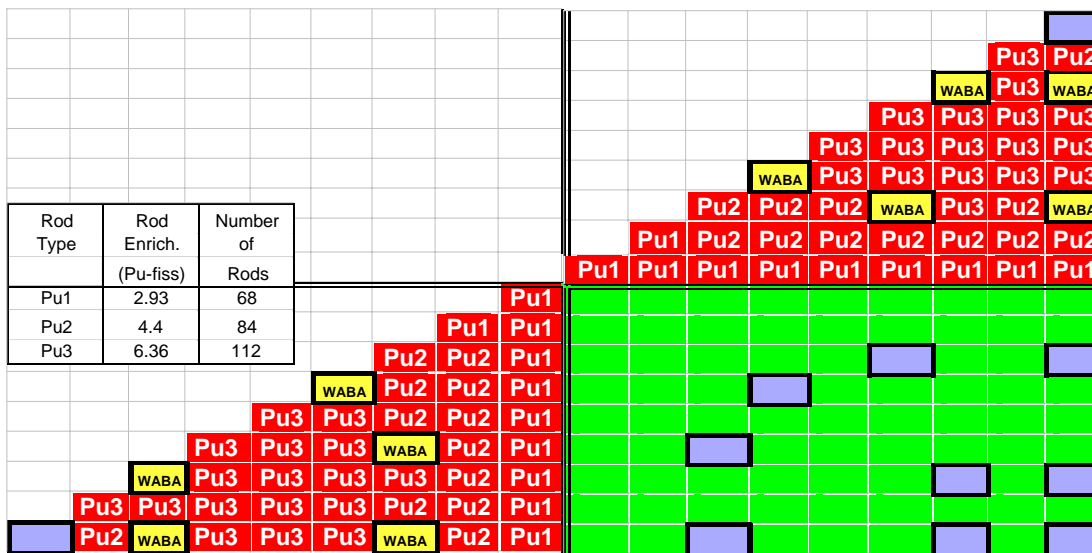


Fig. 4. Optimized enrichment distribution for PWR fuel assembly case.

