

# ***International Workshop on Advances in Applications of Burnup Credit for Spent Fuel Storage, Transport, Reprocessing, and Disposition***

## **Peak reactivity characterization and isotopic inventory calculations for BWR criticality applications**

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**Abstract.** For BWR criticality calculations supporting spent fuel storage racks design, the most reactive fuel assembly to be stored, at its maximum reactivity point (peak reactivity) must be considered.

The determination of the most reactive fuel assembly needs to consider the distribution (as a function of burnup) of the fissile content, burnable absorbers and fission product inventories within the fuel assembly.

BWR fuel designs are highly heterogeneous both radially and axially, with an increasing (in current designs) number of different lattice segments being used, each with its specific enrichment and gadolinium configuration. Moreover, the isotopic evolution (and hence the reactivity) of the BWR fuel also depends on the local core conditions, mainly the coolant void fraction, and control rod insertion histories, during its irradiation life in the core. These characteristics of the BWR fuel make it difficult to define, in a simple bounding way, the fuel characteristics that suit better to criticality analysis production work.

This paper presents a simple conservative method for the definition of the peak reactivity point and isotopic inventory calculation for BWR criticality applications. The relevant parameters considered in this simplified model include the core conditions, gadolinium rod locations, and the initial fissile enrichment distribution as well as the isotopic content for the spent fuel and the axial burnup shape of the fuel assembly. The sensitivity analyses performed make it possible to define a simple yet conservative method to define a fuel bundle material model that can be used in the criticality calculations and that is better suited to criticality analysis production work.

A summary of the sensitivity calculations results are presented, as well as comparisons of the results obtained with the simplified model vs. those obtained with a realistic model of the BWR assembly that confirm the conservatism of the proposed simplified model.

## 1. INTRODUCTION

BWR fuel assemblies use gadolinium rods to control the excess of reactivity at the beginning of life (BOL) of the fuel. In the presence of the gadolinium rods, the evolution of the fuel reactivity with burnup is the result of two opposing effects: on one hand, the reactivity decreases because of the depletion of the <sup>235</sup>U (partially mitigated by the buildup of plutonium fissile isotopes) and the buildup of fission products which absorb neutrons, while, on the other hand, the depletion of the gadolinium absorber increases the reactivity of the fuel. Due to the extremely large absorption cross section of <sup>155</sup>Gd and <sup>157</sup>Gd, the second effect (i.e., reduction of the absorption in the gadolinium) is the predominant phenomenon for the first few MWd/kgU of burnup of the fuel, until the two main absorbing isotopes of gadolinium have almost disappeared (by transmutation to <sup>156</sup>Gd and <sup>158</sup>Gd by neutron absorption).

Therefore, the reactivity of the BWR fuel normally is seen to increase from the fresh fuel case up to a maximum value obtained at a later burnup (hereinafter, referred to as “the gadolinium depletion reactivity peak” or simply “reactivity peak”) that depends on the specific fuel design and on the gadolinium concentration(s) and distribution of the gadolinia fuel rods in the assembly. Beyond this reactivity peak burnup point, the reactivity of the fuel will decrease monotonically with burnup until the fuel is discharged. The “reactivity peak” is the point in life of the bundle that is relevant for criticality analysis purposes, and its characterization and modeling is the object of this paper.

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We will start from the real, complex three-dimensional burned fuel case, the reactivity of which varies point-wise within the assembly depending upon a number of variables (burnup, void fraction, control blade history, axial burnup shape, location of gadolinium rods and  $Gd_2O_3$  concentration, initial  $^{235}U$  enrichment distribution...) and will simplify it in a step-by-step way until a very simple geometrical and material model is developed which envelopes in a conservative manner the real BWR fuel design, with the simplified model based solely on bundle average enrichment and the number and concentration of the gadolinium rods.

## 2. CORE CONDITIONS

As a measure of the reactivity of the bundle all thru this paper we will use the k-infinite value calculated with the standard lattice design code for BWR fuel used in ENUSA. This code is also used to generate the isotopic content of the burned fuel for the subsequent criticality calculations.

As a first step towards developing a simplified BWR bundle design for the criticality calculations, sensitivity analyses were performed to determine the core conditions (how the fuel exposure was accumulated) that lead to the highest value of k-infinite at the reactivity peak. Standard burnup calculations were performed with the lattice physics code, with and without the presence of control rods, at the standard 0, 0.4 and 0.7 coolant void fractions. Following that, a restart at cold uncontrolled conditions was made to simulate the geometry and temperature conditions of the spent fuel pool.

The fuel design used for this analysis is a 10x10 square lattice with 92 fuel rods, and two water rods that occupy an area equivalent to 8 rod cells. Axially, three different lattices (main axial zones) have been considered to take into account the presence of different part length rod designs. Those zones have been identified as BASE, VAN1 and VAN2 lattices. The plenum zones are assimilated to the corresponding VAN lattices. An example of the enrichment and gadolinium rod distribution for the BASE lattice is shown in Figure 1.

	A	B	C	D	E	F	G	H	I	J
1	1.60	2.80	3.60	4.40	4.40	4.40	4.40	3.60	2.80	2.00
2	2.80	4.00	4.40 5.00	4.95	4.40 5.00	4.95	4.95	4.40 5.00	4.95	3.20
3	3.60	4.40 5.00	4.95	4.95	4.95	4.95	4.95	4.95	4.40 5.00	4.40
4	4.40	4.95	4.95	4.95	4.95	WR	-	4.95	4.95	4.95
5	4.40	4.40 5.00	4.95	4.95	4.95	-	-	4.95	4.95	4.95
6	4.40	4.95	4.95	WR	-	4.95	4.95	4.95	4.40 5.00	4.95
7	4.40	4.95	4.95	-	-	4.95	4.95	4.95	4.95	4.95
8	3.60	4.40 5.00	4.95	4.95	4.95	4.95	4.95	4.95	4.95 5.00	4.95
9	2.80	4.95	4.40 5.00	4.95	4.95	4.40 5.00	4.95	4.95 5.00	4.95	3.20
10	2.00	3.20	4.40	4.95	4.95	4.95	4.95	4.95	3.20	2.80

FIG. 1. BWR 10x10 lattice

Figures 2, 3 and 4 represent the calculated cold k-infinite values for the BASE, VAN1 and VAN2 lattice segments. In all three cases the results obtained for the unrodded depletion mode are shown. Additionally, for the BASE case, the results obtained for the rodded depletion mode have been also included.

As shown, for all lattices the highest k-infinite value is reached for the unrodded case when burning at 0% void. This has been repeatedly confirmed many times over several BWR fuel designs covering a wide range of enrichment distributions and gadolinium rod configurations. Therefore, we consider it a general proven rule for criticality analysis-purposes. Note that we are interested only in the k-infinite value at the reactivity peak, and not on the long-term behavior ("burnup credit"), in which case the conclusions would be different.

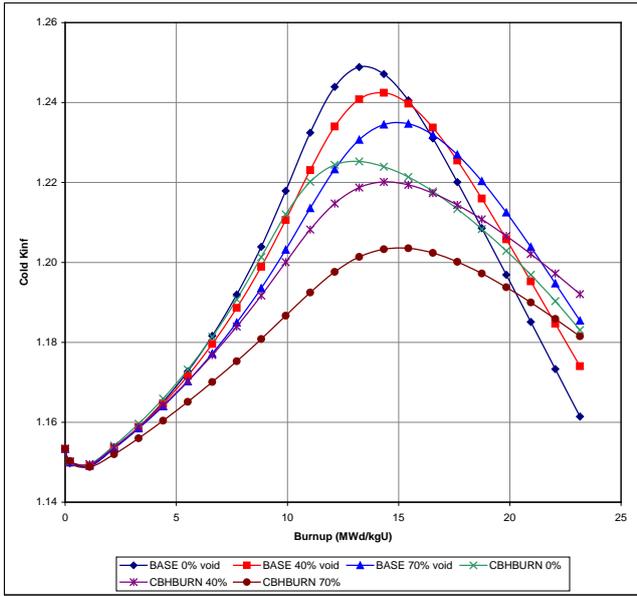


FIG. 2. Cold  $k$ -infinite values for BASE lattice

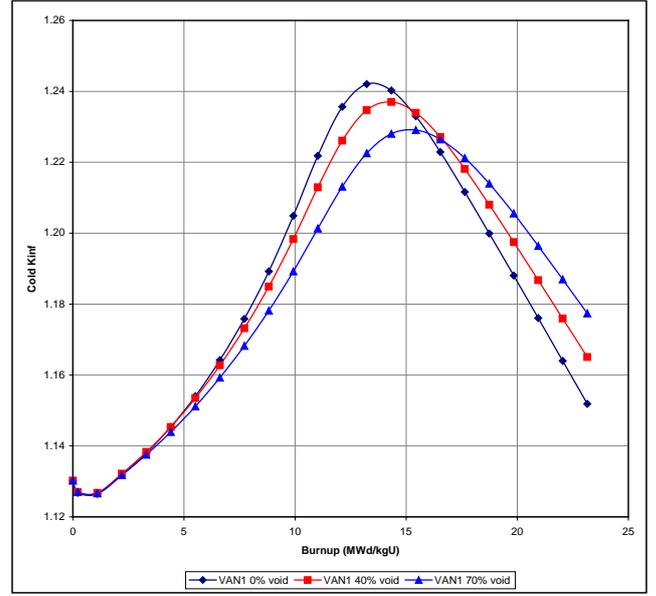


FIG. 3. Cold  $k$ -infinite values for VAN1 lattice

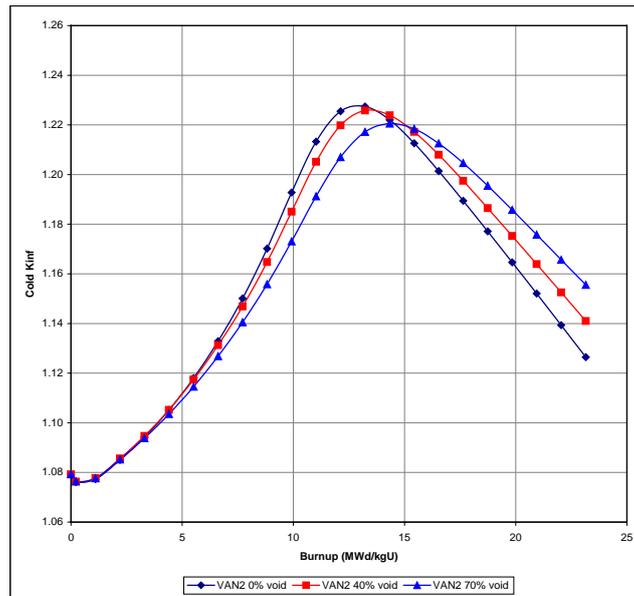


FIG. 4. Cold  $k$ -infinite values for VAN2 lattice

### 3. AXIAL EXPOSURE AND VOID FRACTION SHAPE

Due to the presence of axially varying voids and power, the burnup distribution of a bundle is not uniform axially. For fuel in its first cycle of irradiation, the burnup profile usually has a cosine-like shape, with lower burnup in the bottom and top zones and higher burnup in the central part. An example of this is shown in Fig. 5, where the axial burnup profile obtained at the end of life of an equilibrium cycle at two different locations in the core is shown. These particular assembly positions were selected because their average exposure at the end of their first cycle of irradiation ( $\approx 14.3$  MWd/kgU) corresponds, approximately, to the peak reactivity burnup obtained, after a comprehensive analysis of different core positions, axial exposures and power and control histories, for the same initial enrichment and gadolinium design (number and concentration of gadolinium rods).

The calculated cold k-infinite value is a function of burnup and void fraction as shown in Figures 2 to 4. Therefore, it is possible to obtain “point-wise” k-infinite values for the selected axial burnup and void shapes by interpolating directly in the physics lattice code cold k-infinite tables. These interpolated point-wise k-infinite values can then be compared with the same values obtained considering an axially-uniform burnup shape at 0 void fraction. This comparison has been done at two different exposure steps, namely at 13.23 and 14.33 MWd/kgU that bracket the peak reactivity burnup point for the analyzed bundle designs.

Figure 6 compares the k-infinite values (point-wise burnup and void vs. flat axial burnup profile) for the two bundles selected. The average cold reactivity obtained with the flat profile is seen to yield about 1 to 2% higher cold reactivity values compared to those based on the realistic axial burnup and void shapes.

It is worthy to note that these differences in the bundle cold reactivity are due to differences in the isotopic evolution of the fuel, and these translate, in turn, into differences in the fuel storage rack geometry k-effective of the fuel assembly. Therefore, the flat profile model is conservative for reactivity calculations and thus suitable for criticality analysis of spent fuel.

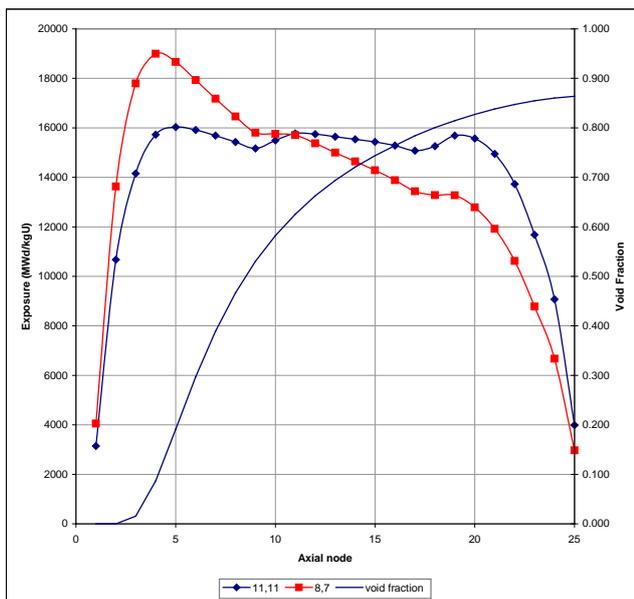


FIG. 5. Axial exposure and void fraction profiles.

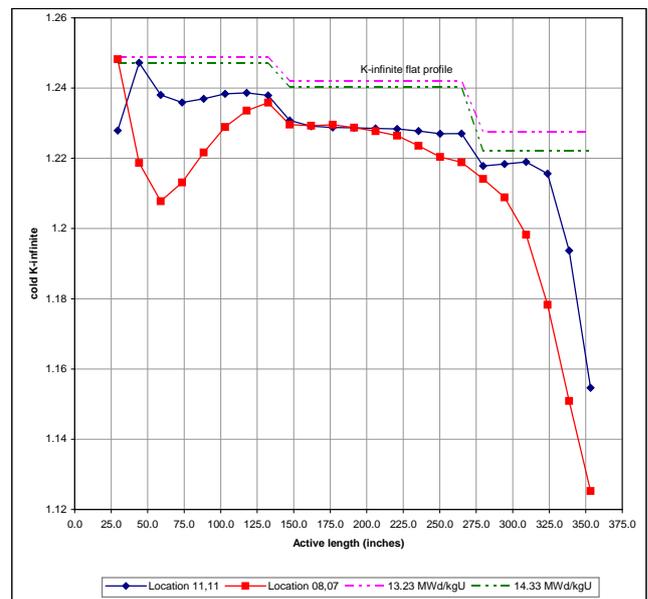
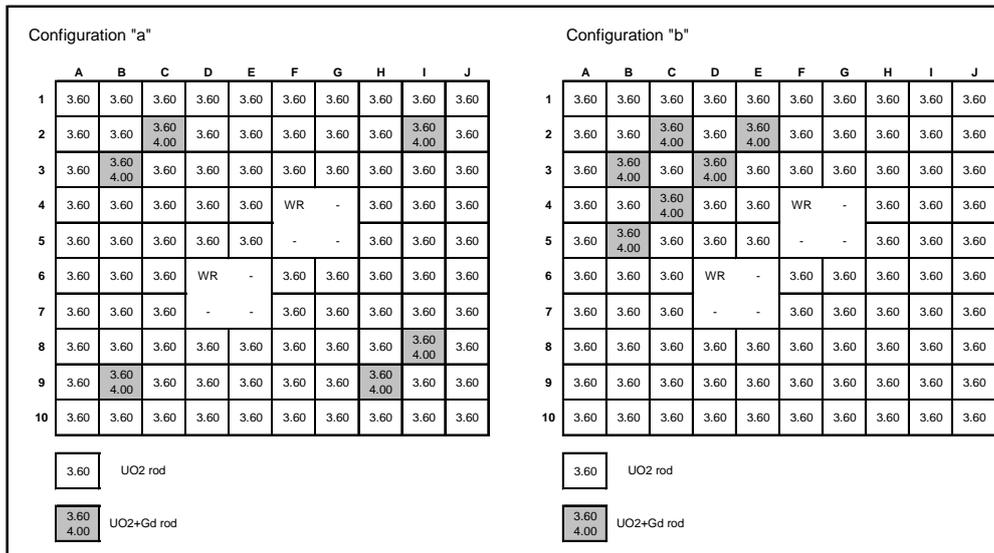


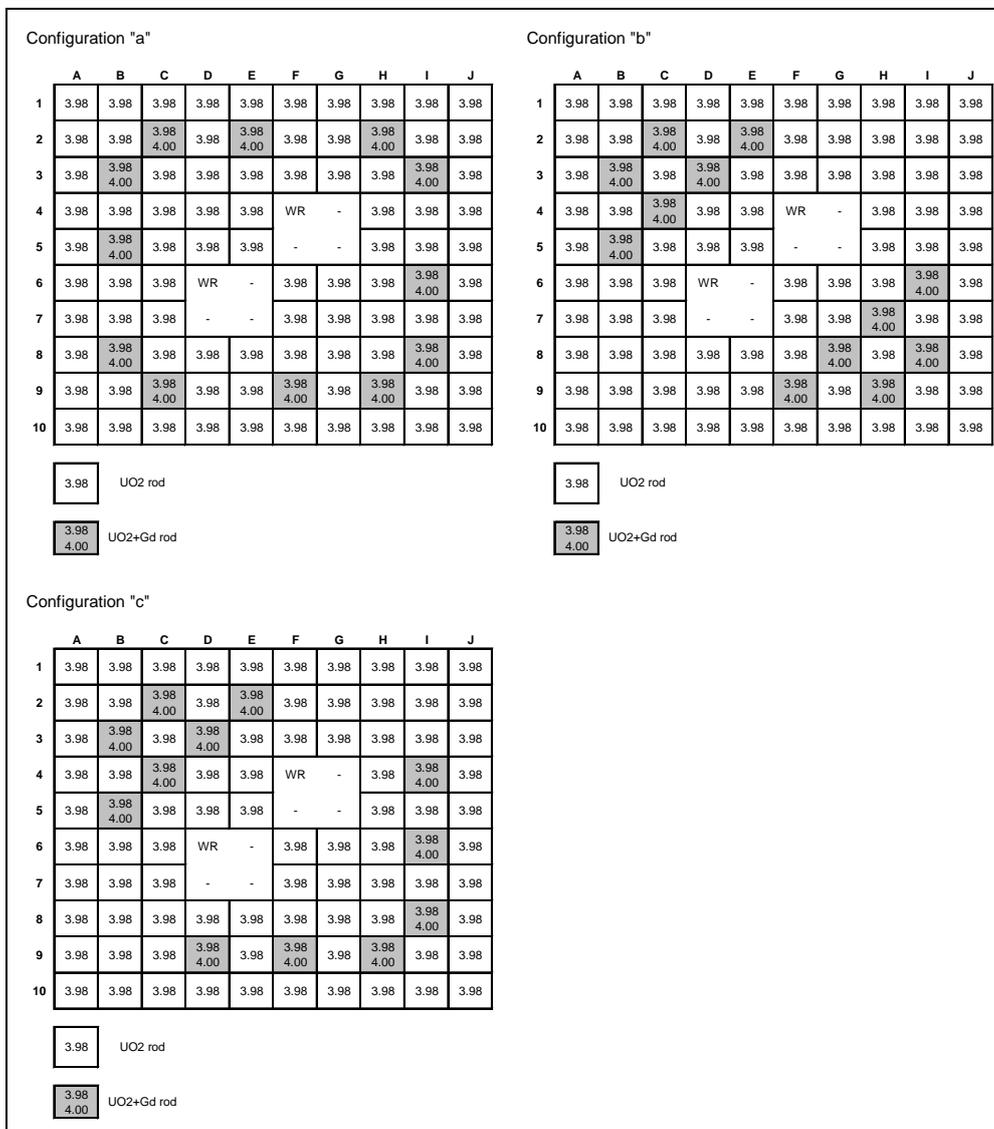
FIG. 6. Axial cold k-infinite profiles

#### 4. GADOLINIUM ROD CONFIGURATIONS

Once the most reactive way of accumulating exposure has been determined, the influence of the position of the gadolinia fuel (Gd) rods inside the lattice is analyzed. Let’s consider different configurations from two different enrichment/gadolinium pairs: a lattice with an enrichment of 3.60%  $^{235}\text{U}$  and 6 Gd rods at 4%, and another one with 3.98%  $^{235}\text{U}$  and 12 Gd @ 4% rods, as illustrated in Figures 7 and 8, respectively. For the moment, we will consider the lattices as being homogeneously enriched, i.e., all rods have the same fissile enrichment. We will address later the effects of the non-homogeneity of the fissile enrichment in the bundle.



*FIG. 7. Gadolinium rods configurations analyzed for 6 Gd 4% rods lattice.*



*FIG. 8. Gadolinium rod configurations analyzed for 12 Gd 4% rods lattice.*

Cold k-infinite values, obtained from the HOTUNC 0% void burnup restart calculations, are shown in Figures 9 and 10. It can be seen that the configuration “a” (with the Gd rods at the outer available positions, and the rods as separated as possible from each other) gives the highest value of the reactivity at the peak reactivity point; while configuration “b”, with the Gd rods closely packed to each others give higher values of k-infinite at BOC, but much lower at the peak reactivity point.

In fact, the configurations that yield the limiting values of reactivity (i.e. maximum value) for the fresh fuel case and at the peak reactivity point are different: the higher is the k-infinite value at BOC, the lower the k-infinite value obtained at the peak reactivity point. The same analysis has been done for several BWR fuel designs obtaining always the same result.

Therefore, for the criticality analysis, the Gd rod locations are chosen to be:

- As closely packed as possible, as in the Figure 7.b for the reactivity calculations for the fresh fuel case. Note that for the case of only a few Gd rods in the bundle ( $\leq 6$  rods) this may be the bounding case, but the depleted reactivity peak configuration needs also to be verified, especially when the bundle only uses 6 Gd rods.
- In the outer zone of the bundle, and with the Gd rod as separated as possible from each other, as in Figures 7.a and 8.a, for lattices whose reactivity peak occurs at an exposure step other than BOC (fresh fuel case). This occurs always for lattices with a loading of Gd rods greater than 6.

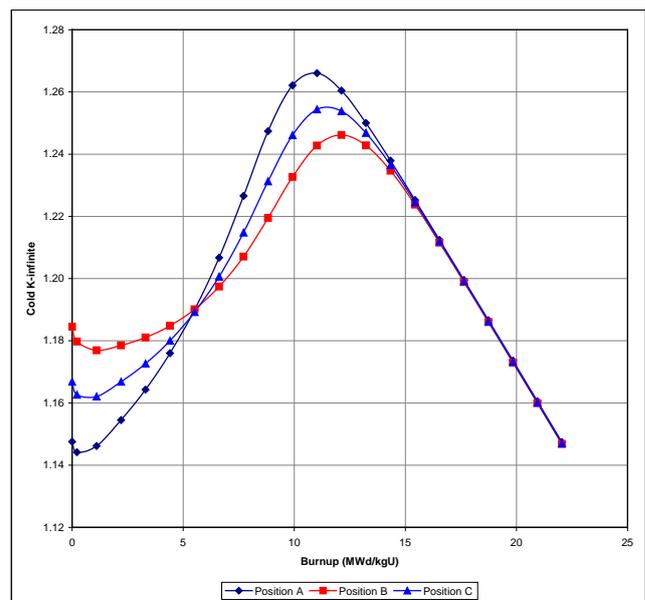
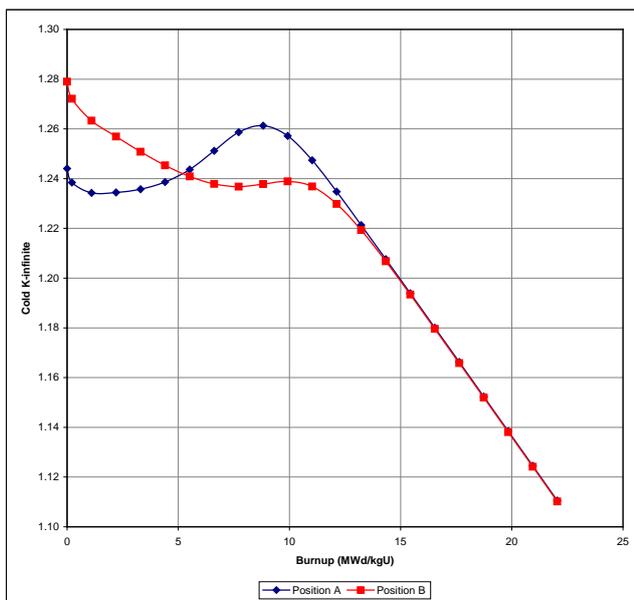


FIG. 9. Cold k-infinite values for 6 Gd4% lattices

FIG. 10. Cold k-infinite values for 12 Gd4% lattices

Different conservative gadolinium configurations selected according to the above criteria are shown in Figure 11. Except for configuration (a) which gives the highest cold k-infinite at BOL, the rest of configurations apply for reactivity peak calculations of burned fuel. Note that no more than 12 Gd rods have been used in the analyses based on the little effect that any additional Gd rod (beyond 12 rods) will have on the k-infinite value of the reactivity peak. Therefore, if more gadolinium is needed to guarantee subcriticality limits for burned fuel, it will be more efficient to increase the concentration of gadolinium rather than the number of rods.

Note that the position of the Gd rods may change for specific designs, mainly due to different PLR locations. Nevertheless, the guidelines governing the selection of the limiting configurations for the criticality analysis will be the same as described above.

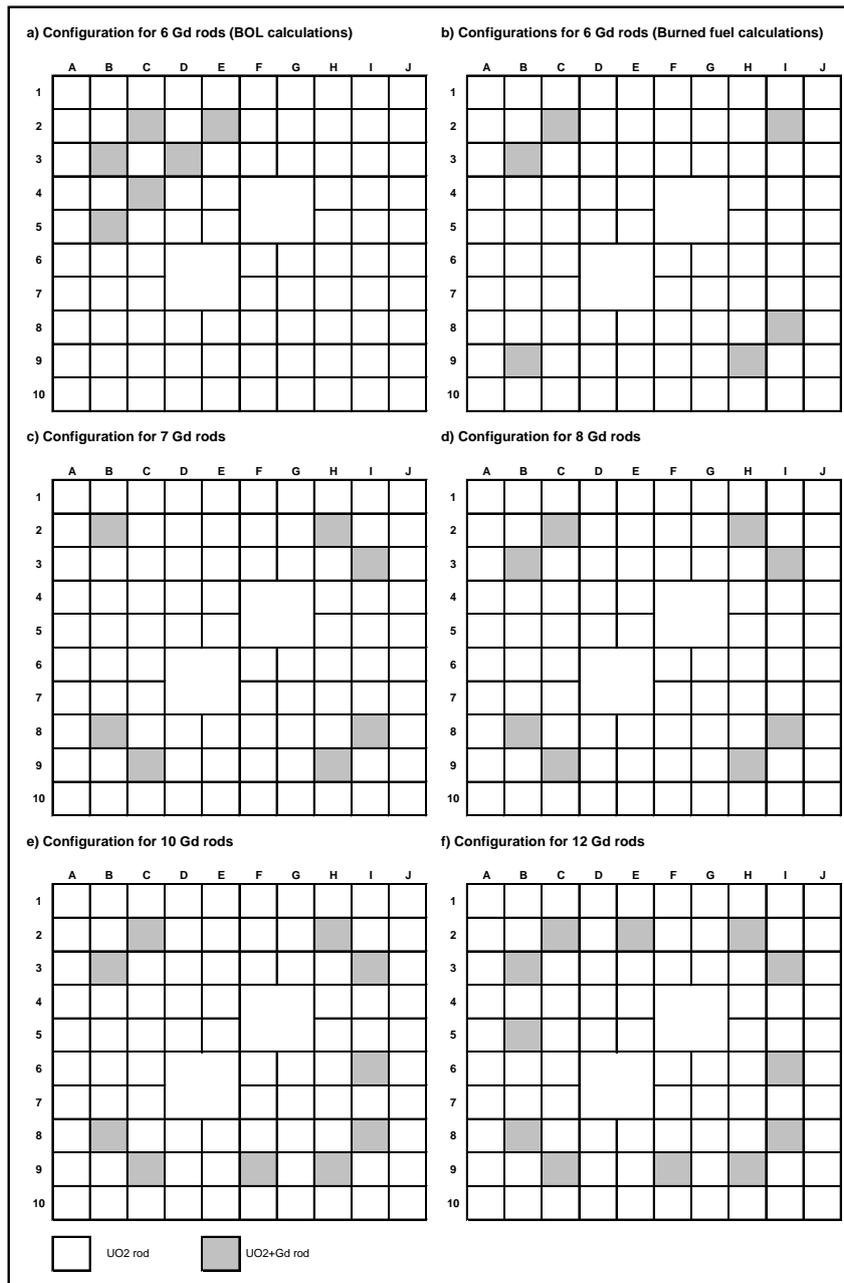


FIG. 11. Conservative Gd rod configurations for criticality analysis

## 5. AXIAL AND RADIAL ENRICHMENT DISTRIBUTION

As commented earlier, the lattice initial enrichment for the fresh fuel case was modeled as being homogeneous. The aim of this section is to demonstrate that this assumption is conservative for the limiting configurations of gadolinium bearing rods for the fresh fuel case.

Fresh fuel can only be limiting for configurations with few gadolinium rods (i.e.,  $\leq 5$  rods) with the rods closely packed together, thus maximizing the Gd rod self-shielding and reducing the gad absorption, as in the bundle design shown in Figure 12 with 5 Gd4% rods. For that case, the average lattice enrichment is 3.748% for the BASE lattice segment, 3.730% for the VAN1 segment and 3.723% for the VAN2 segment. So, the average enrichment of the equivalent homogeneous lattice is:

$$e = \frac{\sum \bar{e}_i \cdot L_i \cdot n_i}{\sum L_i \cdot n_i} = 3.735\%$$

where  $\bar{e}_i$ ,  $n_i$  and  $L_i$  are respectively the average enrichment, the number of rods and the axial length of the lattice  $i$  ( $i$ =BASE, VAN1 and VAN2).

To demonstrate that the homogeneous enrichment case is conservative compared with the real fissile distribution in the bundle, different  $k$ -effective values, assuming heterogeneous and homogeneous radial enrichments, have been calculated using the CSAS25 sequence in SCALE5.1 [1]. The 44 group ENDF/B-V cross-section library has been used for these calculations.

The rack model used for the calculations was a checker-board pattern with one of each two positions occupied by a borated steel tube as shown in the next figure. The model for the homogeneous case was similar except that the fissile enrichment was assumed identical in all rods.

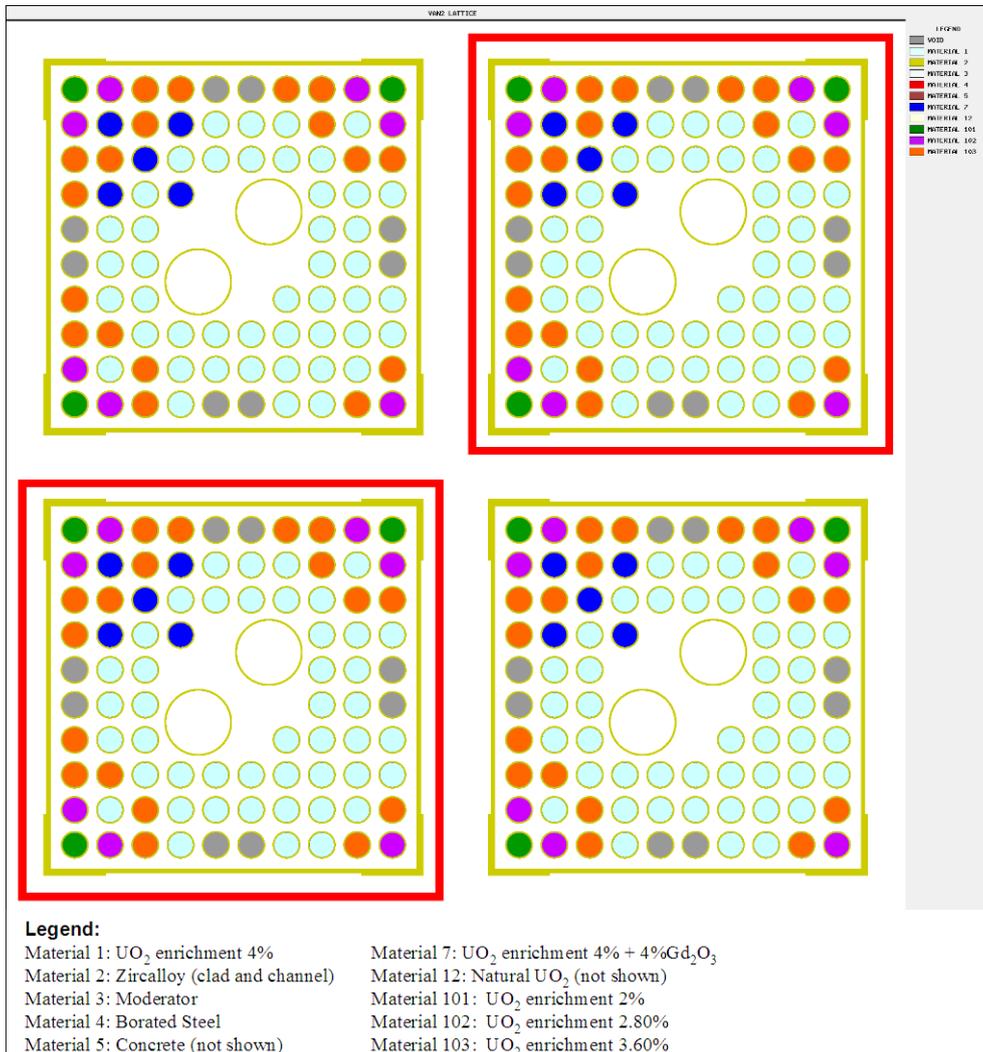


Fig. 12. Heterogeneous enrichment model

The results obtained are shown in Table I. As can be seen the reactivity value for the heterogeneous radial model is almost 1% lower than the one obtained for the simplified homogeneous radial enrichment model in that limiting configuration. Thus, the homogeneous radial model is judged conservative and suitable for criticality analysis.

**Table I. Initial enrichment distribution model results**

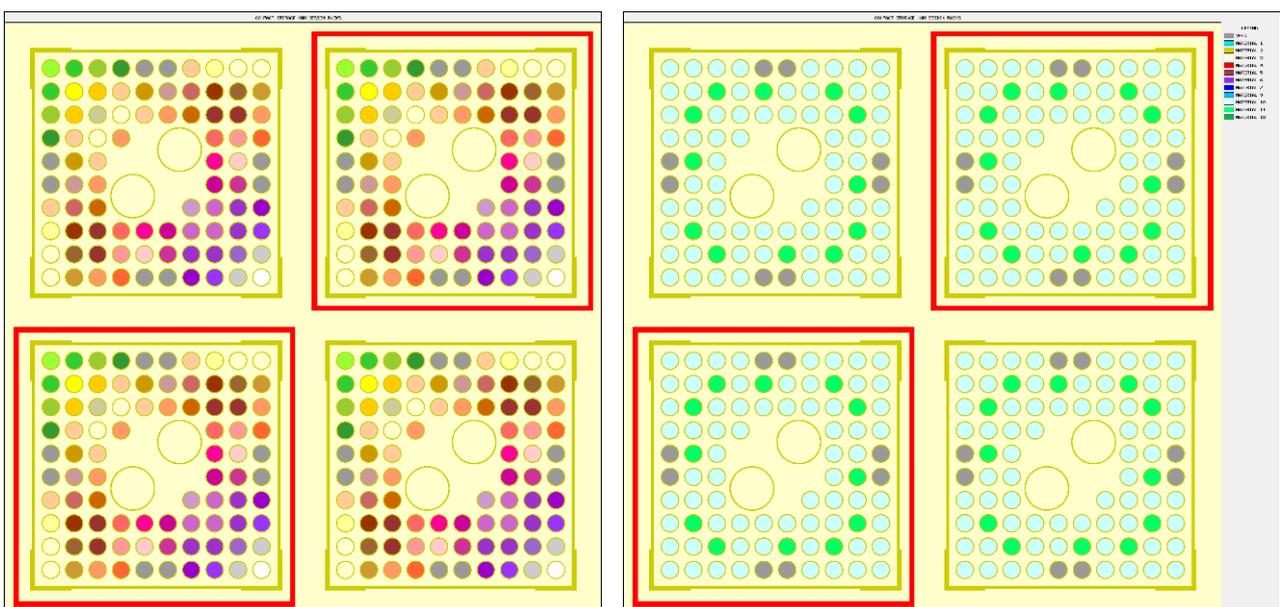
Enrichment model	k-effective	sigma
Homogeneous	0.92564	0.00048
Heterogeneous	0.91766	0.00051

## 6. RADIAL ISOTOPIC DISTRIBUTION

In the previous sections it has been demonstrated that the highest reactivity peak is reached when the lattice is burnt at 0 void fraction without control blades, and that a flat axial burnup shape (i.e., all the axial nodes having the same burnup, accumulated at 0 void fraction) gives a bounding and conservative model of the spent fuel in the criticality calculations.

Therefore, the only variable that remains to be looked at is the rod-by-rod isotopic distribution of the fuel in the radial plane. When the fuel is burnt, the isotopic content is different in each rod, not only due to differences in their initial enrichment but also because their power histories and cumulative exposure are different. Thus, a heterogeneous model of fuel design, like that of Figure 1, will consist, considering the diagonal symmetry of the bundle, of 51 different fuel rods, each one with its corresponding set of isotopic composition for each of the axial segments: BASE, VAN1 and VAN2. Thus, the CSAS25 model needs to consider a total of  $51+47+43= 141$  different isotopic sets (Figure 13).

The lattice code used in this study provides the isotopic content of the fuel both as a bundle average and at the pin-wise detail. Only a set of relevant isotopes from these provided by the lattice code are actually passed to CSAS25. These include the main actinides and some stable fission products, the gadolinium isotopes, and oxygen. In the heterogeneous CSAS25 model, no simplifications are done, and each rod has its proper isotopic content. In the homogeneous model a further simplification is made, which consists in all rods in the lattice segment having exactly the same isotopic content, except for the gadolinium isotopes present in the Gd rods (Figure 14).



*Fig. 13. Heterogeneous radial isotopic distribution Fig. 14. Homogeneous radial isotopic distribution*

The results obtained for the two cases are shown in Table II. The simplified homogeneous radial model gives higher k-effective values than the real heterogeneous design in the peak reactivity range for the limiting gadolinium configurations. This demonstrates that the homogeneous radial isotopic approach is conservative and, hence, suitable for criticality analysis for spent fuel at its peak reactivity point.

**Table II. Homogeneous and heterogeneous bundle model results**

Exposure (MWd/kgU)	Heterogeneous Model		Homogeneous Model	
	k-effective	$\sigma$	k-effective	$\sigma$
12.13	0.90197	0.00047	0.91117	0.00049
13.23	0.90964	0.00048	0.92121	0.00045
14.33	0.90954	0.00058	0.92386	0.00051
15.43	0.90586	0.00052	0.92046	0.00054

## 7. SUMMARY AND CONCLUSIONS

The behavior of the fuel reactivity of spent BWR fuel is analyzed in the storage rack geometry following a step-by-step methodology. The objective of this study is to characterize the reactivity peak in such a way that one is able to model the complex real BWR spent fuel problem by means of a simple and practical conservative model which can be used in production work applications.

Variables that have been considered in the development of this simplified model include: axial void fraction and control rod depletion history, gadolinium rod locations, initial fissile enrichment distribution, axial exposure and void fraction shapes and radial isotopic distribution. Each of these parameters was analyzed separately and a simple model defined bounding the effect of each one. Table III shows the expected range of values for each of the parameters in the real and simplified criticality model where it is apparent the reduction in the range of parameter values that needs to be considered with the simplified model.

The other advantage of the simplified homogeneous criticality model is of a more qualitative nature and is related to the representativeness of the bundle. Note that the concept of “optimum design” for a bundle with fixed average enrichment and number of gadolinium rods is not unique, but doubtlessly some tens of designs will exist that would fulfill all the safety limits of the plant and the energy requirements of the customer. Therefore, the criticality analysis for a real bundle cannot be “generic” in the sense that the real bundle may not be representative of the whole family of bundles with that specified enrichment and loading of gadolinium rods.

On the other hand, the simplified criticality model is by nature “generic”, in the sense that each of the simplifications done is conservative; therefore, when one analyzes a bundle with this model with a specified fissile enrichment and number of Gd rods, that bundle is enveloping and representative of all the bundles with that *average* enrichment (i.e., it does not matter that some rods might have higher enrichments) and number of gadolinium rods or less.

## REFERENCES

- [1] *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, ORNL/TM-2005/39, Version 5.1, Vols. I–III, November 2006. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-732

**Table III. Range of analyzed parameters**

Exposure (MWd/kgU)	Real Model		Criticality Model		
	Parameter	Expected range	# values	Value	# values
	Void fraction	0 - 1	25 <sup>(*)</sup>	0	1
	Control rods	Yes - no	2	No	1
	Gd rods location	Arbitrary	-	Fixed	1
	Axial Exposure	Variable	25 <sup>(*)</sup>	Flat	3 <sup>(**)</sup>
	Initial enrichment distribution	Arbitrary	-	Homogeneous	1
	Spent fuel isotopic radial distribution	Arbitrary	51	Homogeneous	2 <sup>(***)</sup>

(\*) Assuming 25 axial nodes in the standard core calculations

(\*\*) One for each of the BASE, VAN1 and VAN2 zones.

(\*\*\*) One deck for the UO2 rods and the other for the Gd rods.