PERTURBATION ANALYSIS FOR DEMONSTRATION OF REACTIVITY IN CRITICALITY SAFETY ANALYSES

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ABSTRACT

A fissile package assessment per TS-R-1 guidance must be performed assuming that a contents specification provides the maximum neutron multiplication (k_{eff}) consistent with the fuel bundle design and transport conditions. In ensuring demonstration of most reactive and realistic contents specification for licensing criticality safety analyses, a variation of parameters is applied to evaluate the effects on reactivity. Perturbation theory is useful in studying the relative worth of a desired parameter, as it allows determination of the sensitivity of the eigenvalues with respect to changes in the system. This sensitivity analysis results in a simplified contents specification that minimizes any potential, unnecessary restrictions that transport package requirements would impose on the fuel bundle design.

The process of utilizing perturbation theory to determine the most reactive configuration defined by a set of realistic criteria is applicable to criticality safety contents and package evaluations. Through an optimization process, the parameter of effect is chosen, its function and impact investigated, and the relative worth of the parameter is evaluated by application of perturbation theory. Selection of the parameter value is determined by a set of realistic criteria specified by the application. These criteria add realism to the analysis, through basis on actual designs. By selecting the least worth or most reactive parameter value, the package contents can be specified in a manner that ensures maximum k_{eff} consistent with the transport condition.

This perturbation technique is applied to a BWR shipping package criticality safety assessment, which assumes the presence of integral burnable neutron absorber (BA) fuel rods. The effectiveness of the BA rods as a neutron absorber varies with the location of the BA rod within the fuel bundle lattice, and the sensitivity was quantified by the largest present absorber. Package criticality evaluations were performed using the TSUNAMI-3D module in SCALE6 code package, which automates the process of sensitivity and uncertainty analysis. Results justify selection of least worth reactivity locations for BA rods in the BWR lattice, while ensuring a demonstration of most reactive and realistic contents configuration for package evaluations.

INTRODUCTION

A fissile package assessment per TS-R-1 [1] requires a contents specification that provides the maximum neutron multiplication (k_{eff}) consistent with the fuel bundle design and transport conditions. When determining the maximum neutron multiplication, several parameter values, whether unknown or limited by a known range, are evaluated by means of an acceptable variation of the parameter. Perturbation theory is useful in studying the variation of a desired parameter, as it allows determination of the sensitivity of k_{eff} to changes in the package system. This method ensures

determination of maximum k_{eff} while minimizing restrictions imposed on the fuel bundle design, and hence simplifying the contents specification in the package approval document.

Perturbation analysis is applied to criticality safety evaluations of a BWR fuel assembly package that includes evaluations to optimize contents, uncertainty analysis, or validation of calculation methods. The development of analytical perturbation methods is intended for application to validation of calculation methods. The application of these methods to optimize the contents and perform uncertainty analysis extends the use.

The perturbation methods are extended to determine a margin in k_{eff} that is an allowance for material and fabrication tolerances and uncertainties due to limitation in the geometric or material representations used in the computational method. The uncertainty associated with material and fabrication tolerances is quantified by using sensitivity and uncertainty analysis methodology, while the uncertainty associated with geometry or material representations used in the computational model is quantified by using direct perturbation.

METHODOLOGIES

Two methods for the application of perturbation theory are direct perturbation and use of an analytical tool.

Direct Perturbation

Typically, direct perturbation methodology has been used where the parameter of choice is varied and the complete calculation sets are repeated. The direct perturbation method could be used to evaluate the effectiveness of each possible arrangement or parameter variation. The worth of each combination or variation is determined by evaluating the multiplication factor of the nominal system and the perturbed system, as shown in Eq. 1.

Equation 1

$$\rho_{worth} = \frac{k_{\text{nominal}} - k_{perturbation}}{k_{\text{nominal}}}$$

Analytical Perturbation Tool

For some applications, a more efficient methodology uses adjoint-based perturbation theory as an analytical tool to calculate sensitivity coefficients. Calculating the forward and adjoint fluxes allows the calculation of sensitivity coefficients for number densities defining the parameter. The sensitivity coefficients are calculated using the SCALE sensitivity and uncertainty (S/U) analysis tool TSUNAMI-3D, which utilizes the Monte Carlo computer code KENO-VI [2].

Validation of Analytical Perturbation Tool

When using an analytical tool it is necessary to validate the results. Hence the energy-integrated sensitivity coefficients, computed by TSUNAMI, are validated through the use of central difference direct perturbation sensitivity calculations. Through this technique, the sensitivity of k_{eff} to the number density of particular nuclide can be obtained. This sensitivity of k_{eff} to the number density is equivalent to the sensitivity of k_{eff} to the total cross section, integrated over energy. Because the total cross section sensitivity coefficient tests much of the data used to compute all other sensitivity coefficients, it is considered an adequate test for verification. For each sensitivity coefficient examined by direct perturbation, the k_{eff} of the system is computed first with the nominal values of

the input quantities, then with a selected nominal input value increased by a certain percentage, and then with the nominal value decreased by the same percentage. Often when computing three-dimensional calculations, it may not be possible to meet both the linear behavior and 15-standard-deviation spread criteria defined in the code manual [2]. In such cases, it may be necessary to use more sophisticated techniques or to accept a qualitative verification. It is important in sensitivity calculations to ensure that the k_{eff} value of the forward and adjoint solutions closely agree. If the k_{eff} values do not agree, then the quality of at least one of the transport calculations may be in question.

APPLICATIONS

Both direct and analytical perturbation methods are applied in optimizing the burnable absorber rod arrangement and uncertainty allowance analysis.

CONTENTS SELECTION: BURNABLE ABSORBER RODS

Burnable absorber rods within a BWR assembly are utilized to achieve desired core performance objectives, extending the life of the fuel bundle during the power generation cycle, by varying the number, arrangement, and gadolinia-oxide content in the fuel rods. As a neutron absorber, the location of the rod in the bundle is significant to the reactivity of the BWR bundle shipping package.

Burnable Absorber Rod Evaluations

The evaluation process consists of an optimization step that assesses each viable BA rod location in the bundle by sensitivity analysis through implementation of perturbation theory and then an evaluation of selected BA rod patterns by validation and verification. This process ensures that the most realistic and reactive contents, defined by constraints, are specified for criticality safety evaluations of the fuel contents and packaging to demonstrate the maximum k_{eff}.

The models are defined as an infinite array of fuel bundles as to represent the package array with each fuel rod evaluated at 5.0 weight-percent (wt%) enriched UO_2 fuel containing a small quantity of 0.1 wt% Gadolinia oxide (Gd_2O_3). The small amount of Gd_2O_3 allows calculation of a relative sensitivity coefficient without introducing a large perturbation of the flux in the fuel lattice. It is important to note that for neutron absorbers/poisons, the absorption characteristic is too strong to allow for meaningful estimates of the absolute burnable absorber worth; hence, to evaluate the BA rod worth in every viable location, the rods are characterized by relatively weak absorption by using a small quantity of gadolinia oxide, as to not alter the flux characteristic of the bundle. ^{155}Gd and ^{157}Gd have the largest thermal neutron capture cross sections. ^{157}Gd is used to trace the sensitivity coefficients because of its large thermal neutron cross section. Within the SCALE input, each fuel rod and material is described by a unique material identifier; this allows for the code to perform flux calculations for each rod location within the lattice so that individual location effects are accounted for.

Sensitivity coefficients and their associated statistical uncertainties integrated over energy and region for ^{157}Gd are utilized to evaluate least worth Gad rod locations within the evaluated bundle. Sensitivity coefficients of ^{157}Gd from TSUNAMI-3D calculations were mapped in the modeled bundle configuration. Figure 1 shows the ^{157}Gd worth on a BWR 10x10 bundle map, where yellow represents the greatest worth location, red represents the least worth location (i.e., Gad rod has the smallest sensitivity coefficient), and varying shades of orange represent the worth gradient between yellow and red.

A	B	C	D	E	F	G	H	I	J	
20	19	18	17	16	15	14	13	12	11	1
30	29 -2.2832E-03	28 -1.9420E-03	27 -1.9970E-03	26 -2.5205E-03	25 -2.6090E-03	24 -1.9613E-03	23 -1.9569E-03	22 -2.2919E-03	21	2
40	39 -1.9138E-03	38 **-1.6502E-03**	37 **-1.7774E-03**	36 -2.7852E-03	35 -2.6734E-03	34 **-1.8492E-03**	33 **-1.6404E-03**	32 -1.9248E-03	31	3
50	49 -1.9415E-03	48 **-1.8267E-03**	47 -2.7053E-03	46	45	44 -2.8217E-03	43 -1.8826E-03	42 -1.9808E-03	41	4
60	59 -2.5325E-03	58 -2.6794E-03	57	56	55	54	53 -2.7371E-03	52 -2.5971E-03	51	5
70	69 -2.5999E-03	68 -2.8032E-03	67	66	65	64	63 -2.8647E-03	62 -2.6076E-03	61	6
80	79 -1.9551E-03	78 -1.8649E-03	77 -2.8835E-03	76	75	74 -2.6898E-03	73 **-1.8627E-03**	72 -1.9603E-03	71	7
90	89 **-1.8588E-03**	88 **-1.6393E-03**	87 -1.8683E-03	86 -2.7777E-03	85 -2.7629E-03	84 **-1.7999E-03**	83 **-1.6416E-03**	82 -1.9201E-03	81	8
100	99 -2.3131E-03	98 -1.9008E-03	97 -1.9490E-03	96 -2.5318E-03	95 -2.5503E-03	94 -1.9825E-03	93 -1.9316E-03	92 -2.2942E-03	91	9
110	109	108	107	106	105	104	103	102	101	10

Figure 1. ^{157}Gd worth BWR bundle map

Utilizing the results, as mapped in Figure 1, a set of BA rod locations is chosen taking into consideration BA rod worth and constraints on viable BA rod locations, based on fuel designs. In general, the lower worth BA rods are found in lattice locations furthest from moderated regions (water hole, water channel or edge of lattice). Performing the package contents assessment using the perturbation theory techniques and applying less restrictive, more realistic criteria to specify the package contents is an important tool in more efficiently defining and validating the maximum neutron multiplication factor.

Validation of Analytic Perturbation Application

Validation of the analytical tool, as used to evaluate the sensitivity of the BA rod locations, is achieved through direct perturbation of the material number density, as this application is equivalent to the uniform perturbation of the total cross-section across all energy groups. Two models, representing the application of the BA rod patterns to the multi-package analysis, are utilized: infinite single rod array and an infinite bundle array (as used in the BA rod worth evaluation). All models utilize an actual Westinghouse BWR fuel design. The direct perturbation is only applied to ^{157}Gd, since the relative worth of that isotope is evaluated when selecting the least worth BA rod locations. The perturbed difference is scaled for linear comparison to avoid asymmetric result.

Direct perturbation results are shown in Table 1 for each of the comparison cases. The number density multiplier signifies the value change applied to the ^{157}Gd isotope. Various number density multipliers are evaluated until linearity is ensured. The nominal number density multiplier of 1 represents the TSUNAMI result, and is the basis for the sensitivity coefficient comparison. Within the table, the Notes column displays messages for acknowledgement. Although the comparisons are greater than 15 standard deviations (std dev) apart, the k_{eff} values of the forward and adjoint calculations closely agree for each case, within the code acceptance criteria. The sensitivity and

uncertainty columns display the direct perturbation calculation results of the sensitivity coefficient and the associated combined uncertainty. Comparing the direct difference sensitivity coefficients between the nominal (TSUNAMI) and perturbed result, the percent difference displays the relative closeness of the sensitivity coefficients and the calculation methods.

Table 1. Direct Perturbation Validation Results

Case	Number Density Multiplier	k_{eff}	Sigma (σ)	DP Sensitivity Coefficient ($S_{k,\alpha}$)	DP Sensitivity Uncertainty (σ_s)	Sensitivity Coefficients Percent Difference (%)	Notes
Fuel Rod	1 - nominal	1.00358	0.00025	-0.18949	0.00025	--	--
	1.013	1.00071	0.00027	-0.20082	0.00122	6.0	> 15 std dev apart
	0.987	1.00595	0.00035				
	1.1	0.98500	0.00028	-0.19216	0.00038	1.4	>15 std dev apart
	0.9	1.02357	0.00027				
Infinite Bundle Array	1 - nominal	1.11270	0.00130	-0.11529	0.00130	--	--
	1.1	1.09850	0.00120	-0.12762	0.00115	10.7	> 15 std dev apart
	0.9	1.12690	0.00120				

NOTE: direct perturbation (DP)

Verification of BA rod Patterns by Direct Perturbation

Verification of BA rod patterns is evaluated by direct perturbation of varied BA rod patterns. Examination of various patterns tests the selection criteria used to define the set of BA rod locations that were chosen to demonstrate maximum credible reactivity for the contents. Four different patterns were evaluated, as follows (shown in Figure 2):

- Pattern #1: eight BA rods in three quadrants, symmetric about the major diagonal
- Pattern #2: top eight least worth rod positions
- Pattern #3: top four least worth pairs
- Pattern #4: eight BA rods in four quadrants, symmetric about the major diagonal

Utilizing the ^{157}Gd sensitivity coefficients to quantify the worth of each rod position, the various patterns are determined by the BA rod selection process. Pattern #1 is the resultant BA rod pattern recommended by BA rod analytical perturbation and selection criteria as suitable for defining the most reactive contents specification. Patterns #2 through #4 are essentially the steps used to arrive at the resultant pattern, Pattern #1, and show how the addition of realism in the selection criteria can change the system reactivity. Pattern #2 represents the top eight least worth BA rod positions in the bundle. To apply the rule of symmetry about the major diagonal, the averages of equivalent rods or pairs across and along the major diagonal are quantified. Then the pairs are categorized by their least worth average specified per quadrant. Pattern #3 is the selection of the top four least worth average of pairs, implying symmetry is already applied and no quadrant criterion is enforced. Pattern #4 is similar to Pattern #3, although the criterion of a BA rod in each of the four quadrants is applied. Depending on the fuel design Patterns #3 and #4 may be interchangeable. As seen in

Figure 2 for the BWR fuel, where the top least worth rod pairs occur in all four quadrants, and hence only the upper-left quadrant pair is shifted to the major diagonal for comparison.

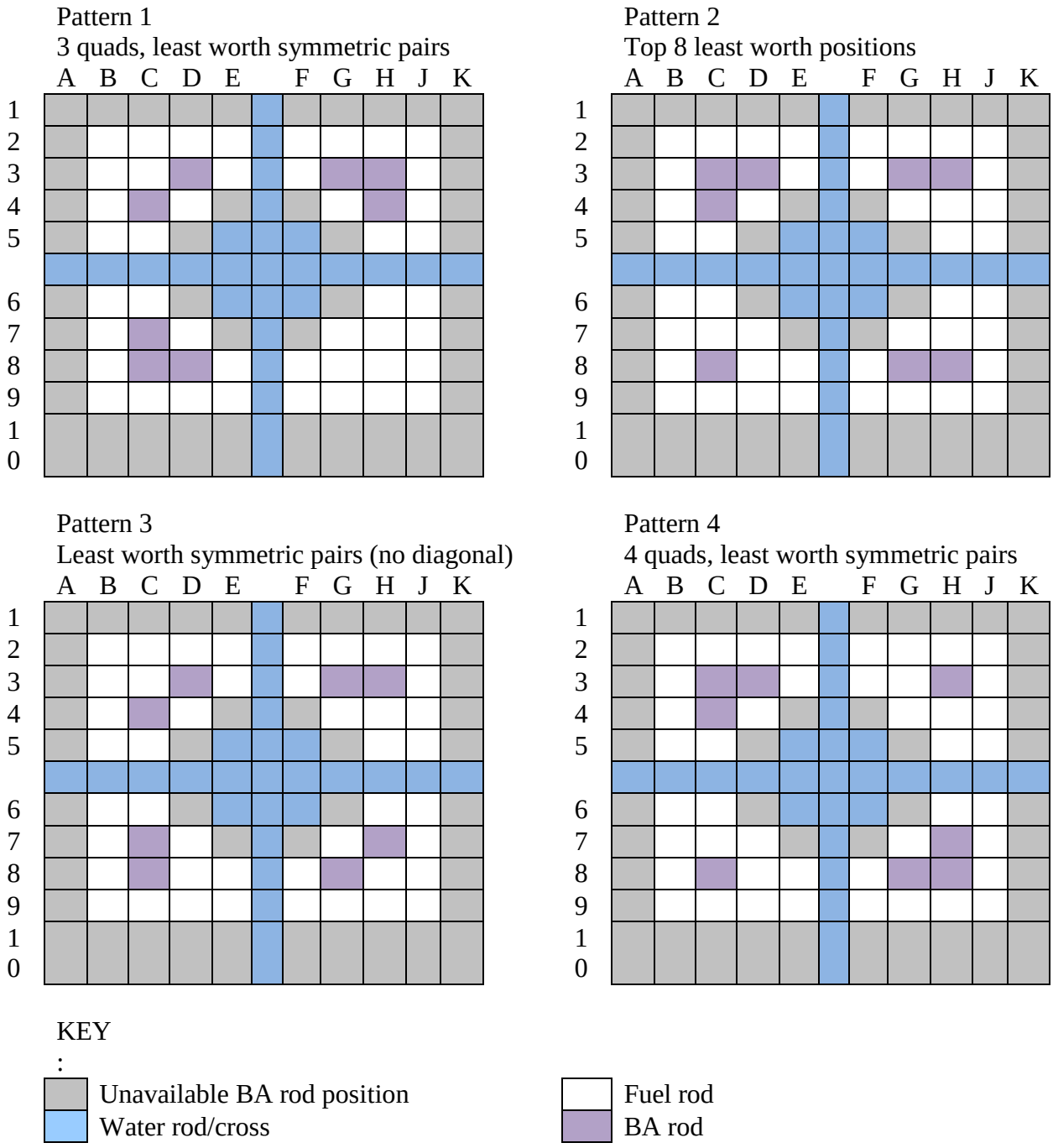

Figure 2. Variation of SVEA BA Rod Patterns for Verification

Results shown in Table 3 display the system reactivity of each BA rod pattern in the infinite array case. Each pattern represents a step of the BA rod selection process, as utilized to apply constraints for determining the most reactive fuel contents. Pattern #1 is the application of all selection criteria and constraints recommended for demonstration of the most reactive contents and, as shown in

Table 3, exemplifies the most reactive contents specification. It should be noted that Pattern #4 is within two sigma of the Pattern #1 selection, and hence are statistically the same value. Comparison of pattern results shows that k_{eff} is not particularly sensitive to the applied constraints in the BA rod selection process. Therefore, there is no significant uncertainty associated with the selected least worth BA rod patterns and constraints for most reactive package contents with credited BA rods.

Table 3. Results of Verification by Direct Perturbation

Fuel	Pattern	k_{eff}	sigma	Description	
BWR 10x10 lattice	#1	0.60473	0.00085	Pattern #1	3 quads, least worth symmetric pairs
	#2	0.60301	0.00099	Pattern #2	Top 8 least worth positions
	#3	0.59535	0.0008	Pattern #3	Least worth symmetric pairs (no diagonal)
	#4	0.60592	0.00086	Pattern #4	4 quads, least worth symmetric pairs

UNCERTAINTY SENSITIVITY ASSESSMENT

Allowance for other uncertainties (Δk_u) includes two uncertainty categories: (1) material and fabrication tolerances and (2) geometric or material representations used in the computational method. The uncertainty associated with material and fabrication tolerances is quantified by using a sensitivity and uncertainty analysis methodology, which is the application of perturbation theory by use of the analytical tool. Direct perturbation is used to quantify the uncertainty associated with geometry or material representations used in the computational model.

Material and Fabrication Tolerances

The effectiveness of a material at suppressing reactivity in the transport system is dominated by its absorption reaction rate. The absorption reaction rate of a material can be determined using the following equation:

Equation 2

$$R = \phi\Sigma = \phi N\sigma$$

Where:
R = absorption rate in absorptions/cm^3-s
ϕ = neutron flux in n/cm^2-s
Σ = macroscopic cross section in absorptions/cm^3
σ = absorption cross section in cm^2
N = Number Density in atoms/cm^3

This equation shows that the reaction rate is proportional to both the absorption cross section and the number density of the material of interest. Therefore, an equivalent change in either number density or absorption cross section will result in the same percentage change in reaction rate. Additionally, the number density changes proportionally with the material density, and relates the material density to the reaction rate, yielding Eqs. 3.

Equation 3

$$\Delta N = \frac{N_A}{M}\Delta\rho$$

$$\Delta R = \phi\frac{N_A}{M}\Delta\rho\sigma = \phi N\Delta\sigma$$

The equation above demonstrates that the reaction rate of a material, and therefore its relative effect on system reactivity, will change by the same amount given an identical percentage change in either material density or absorption cross section. TSUNAMI has been used to define the change in reactivity for a system on a 1% change in cross section basis for a given material. The change is defined as the sensitivity coefficient of the material, $\Delta k/k/\Delta\Sigma/\Sigma$, which then can be related to changes in either cross section or material density as specified in Eq. 4.

Equation 4

$$\frac{\Delta keff/keff}{\Delta\Sigma/\Sigma} = \frac{\Delta keff/keff}{\Delta\rho/\rho} = \frac{\Delta keff/keff}{\Delta\sigma/\sigma}$$

For the tolerance values being studied in this system, the reactivity affect on the system must be determined based on a change in the total amount of the material of interest present. This can be accomplished in one of two ways:

- Study of an explicit change in material volume due to tolerance value
- Study of a change in material density proportional to the volume change assuming constant volume to match the volume based material change

As the geometric differences between the materials being studied are small compared to their total size in the system, it is reasonable to assume that a small change in material density will produce equivalent reactivity effects as a change in the material volume. In other words, a change in thickness of a material is effectively the same as a change in density for a fixed volume of the same material. This conservation of mass assumption can be written as:

Equation 5

$$-\frac{\Delta V}{V} \equiv \frac{\Delta\rho}{\rho}$$

Likewise, the sensitivity to total cross section is also equivalent to the sensitivity to material thickness provided the material is associated with a material region of approximately the same thickness. The effect of the uncertainty in material properties on k_{eff} can be estimated by multiplying the sensitivity coefficient for each material by a relative uncertainty in the material density or volume.

The uncertainty associated with each material region is calculated using the relative change in volume $\Delta V/V$ for the geometry of the region. The individual relative uncertainties are combined as a simple summation, not taking credit for the possibility of the uncertainties being independent of each other by using a statistical sum. This results in a conservative estimate of the uncertainty as

the simple sum ignores the possibility that the material tolerances are independent of each other. Equations to relate changes in volume to applicable geometries and tolerances being studied are presented later in this section.

Equation 6

$$\left(\frac{\Delta keff}{keff}\right)_i = \left[\frac{\Delta keff/keff}{\Delta\Sigma/\Sigma}\right]_i \cdot \left(\frac{\Delta V}{V}\right)_i$$

$$\left(\frac{\Delta keff}{keff}\right)_{TOTAL} = \sum_i \left(\frac{\Delta keff}{keff}\right)_i$$

The total absolute uncertainty associated with the material tolerance, Δk_u, is obtained by multiplying the relative uncertainty by k_p =1.0 with the assumption that $\Delta k_{eff}/k_{eff}$ is independent of the absolute value of k_p that is calculated for the package system.

Equation 7

$$\Delta k_u = \left(\frac{\Delta keff}{keff}\right)_{TOTAL} \times \quad k_p \quad \text{where } k_p = 1.0$$

Uncertainties based on material tolerances are related to the changes in volume based on the applicable geometric equation. The relative change in volume for a solid cylindrical geometry, such as fuel pellets, is two times the relative change in radius.

$V = \pi h r^2$

where

h = height of the material

r = average radius of the material

$dV = 2\pi\, h\; r\, dr$

where h is constant

$$\frac{dV}{V} = \frac{2\; r\, dr}{r^2}$$

$dr = \omega\, r$

where ω is the tolerance for r

$$\frac{dV}{V} = 2\;\omega$$

For example, a 0.2 percent tolerance on radius is a 0.4 percent change in volume.

Geometric or Material Representations

The effect of packaging materials or dimension such as inner container spacing within the outer container, outer container dimension, and polyethylene foam cushion redistribution are evaluated by comparing the nominal package configuration to the perturbed package configuration. The perturbed configuration is the result of realistic rearrangement that results from credible accident conditions (impact or fire).

The effect of a change in geometric or material representation is calculated as the difference between the nominal and perturbed case:

Equation 8

$$\Delta k = k_{perturbed} - k_{nominal}$$

For example, spacing between packages in an array is increased and decreased to determine the effect of k_{eff} in the package evaluation. The nominal spacing is defined as close packing allowed by the nominal dimensions of the outer container. The spacing between packages may increase due to transport conditions (normal arrangement on conveyance or rearrangement during an impact). Damage to the outer container may decrease the spacing allowed between packages. Increase in spacing results in a decrease in k_{eff} where as a decrease in spacing results in an increase in k_{eff}. For a 2.5 in decrease in spacing the following Δk and hence uncertainty change may be determined as follows:

$\Delta k = k_{-2.5\ in} - k_{nominal} = 0.88532 – 0.86997 = 0.01535$

CONCLUSIONS

Expanding the application of perturbation theory and the use of sensitivity and uncertainty analysis methodology to contents selection and uncertainty analysis allowed the maximum neutron multiplication factor for the package assessment to be more efficiently defined, hence simplifying the contents specification in the package approval document.

Use of the analytical perturbation method for evaluating BA rod position worth in a BWR lattice was shown as a valid method of optimizing the contents parameters. In addition, the analytical perturbation method facilitated a more thorough understanding of the lattice physics.

Development of the uncertainty methodology for quantifying package assessment uncertainty allowances as based on sensitivities from analytical and direct perturbation methods shows direct connection between the changes is system neutron multiplication to the change in nuclide density. Further evaluation to validate the relationship between the relative change in volume and change in k_{eff} is being conducted.

REFERENCES

1. IAEA Safety Standards Series, TS-R-1, Regulations for the Safe Transport of Radioactive Material, 2009 edition
2. “SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation,” NUREG/CR-0200, ORNL/TM-2005/39, Version 5.1, Vols. I–III, CCC-732, Radiation Safety Information Computational Center (2006).