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Summary

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**A Statistical Method for Estimating the Net Uncertainty in the
Prediction of k Based on Isotopic Uncertainties**

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A Statistical Method for Estimating the Net Uncertainty in the Prediction of k Based on Isotopic Uncertainties

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Introduction

Validation of burnup credit methodologies requires that any biases and uncertainties in the ability to predict isotopic concentrations be determined by comparison between calculations and measured data. However, the approach used in applying nuclide biases and uncertainties to obtain a conservative estimate of the neutron multiplication factor for a spent fuel configuration is not defined in any regulatory guidance or standard. Currently, the approaches proposed by the U.S. Department of Energy in Topical Reports submitted to the U.S. Nuclear Regulatory Commission take a very conservative approach by assuming all nuclides are at statistical extremes simultaneously. In other words, given biases and uncertainties determined from the comparison of calculated and measured data for a set of nuclides, the calculated concentrations for each nuclide are corrected by applying the bias, the uncertainty, and a multiplier on the uncertainty, so as to maximize predictions of fissile nuclides and minimize those of absorbers. In practice, however, the key parameter of interest is the neutron multiplication factor, k , for a

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given spent fuel system, to ensure an adequate subcritical margin. This summary describes an approach whereby it is possible to estimate the uncertainty in k directly with respect to biases and uncertainties in individual nuclide concentrations, while maintaining a high degree of confidence in the calculated result.

Theory

In the calculation of k_{eff} for a spent fuel system, nuclide concentrations are first estimated using a depletion method. Using measured (M) and corresponding computed (C) isotopic concentrations for each nuclide and for n measurements, one can calculate an average measured-to-computed ratio for nuclide i as:

$$\bar{X}_i = \sum_{j=1}^n (M_{i,j}/C_{i,j}) / n .$$

The standard deviation of this ratio is simply the statistical deviation of the individual M/C ratio for each of the n measurements. \bar{X}_i can be considered to be a multiplicative bias for nuclide i , where the best estimate of a future measured concentration M^* is obtained from the calculated concentration C^* by $M_i^* = C_i^* \times \bar{X}_i$. This statistical procedure is discussed in detail in Ref. 1; a summary of the procedure and statistical results based on 38 sets of chemical assay measurements are presented in Ref. 2.

For a future measurement, the value of M^* would be expected to lie in the range $C^* \times (\bar{X}_i \pm T_n \cdot s)$, where T_n is a tolerance factor determined for n measurements, at a given confidence level (also detailed in Ref. 1), and s is the standard deviation. Thus, for any given fuel sample with a set of computed isotopic concentrations, one can determine the range of

expected values of each isotope. The statistical confidence in that range is determined by the choice of the tolerance factor. The conservative approach described earlier sets fissile nuclides to the maximum of the range, and non-fissile absorber nuclides to the minimum of the range, where the range itself is determined on a nuclide by nuclide basis. In reality, we would expect actual fuel nuclide concentrations to vary in a random fashion, normally distributed around a mean, relative to bias-corrected calculated concentrations. The random deviations result from modeling uncertainties, operational variations, design uncertainties, and other factors.

In setting calculated concentrations to their conservative limits, one is confident that one can conservatively estimate the reactivity of the burned or spent fuel. However, if one were to randomly vary spent fuel isotopics independently within their expected ranges, calculate the neutron multiplication factor, k , for a given fuel configuration, and repeat this process multiple times, one would obtain a normal distribution of k values corresponding to random variations in expected concentrations. The distribution itself will have a standard deviation, which can be used to set a confidence level on the prediction of k .

Approach

In order to converge on a statistically meaningful value of k for a given configuration, a large number of independent calculations is necessary. To serve this need, the computer code CHRONOS (Calculation of Homogenized Reactivity of Nuclides with Omni-Sampling) was developed to automate the process of setting up, executing, and parsing the output of a large number of independent calculations with the CSAS1X sequence of SCALE³ (infinite-lattice XSDRNPM calculations). To study the effect in a cask environment with inclusion of the axial

burnup distributions, a subsequent version, KRONOS, was developed to perform the same procedure with three-dimensional KENO⁴ models. Both systems were compiled using MPI (Message Passing Interface)⁵ to allow simultaneous execution of a number of calculations on a distributed network, and thus improve turnaround time.

Calculations performed to-date are based on a set of 1000 sets of criticality calculations. In each calculation, all actinide and fission product concentrations are varied simultaneously. Results show that calculations converge to a fixed standard deviation (representing a well-characterized normal distribution) within 500–700 criticality calculations. Figure 1 shows the convergence of the standard deviation for one of the cases analyzed, and Figure 2 illustrates the distribution of k_{eff} values about a mean for the sets of calculations performed for this burnup state. The mean and standard deviation (0.9523 " 0.0078) associated with Figure 2 serve to characterize the mean k_{eff} value and uncertainty as a function of isotopic biases and uncertainties, for the geometry and burnup modeled.

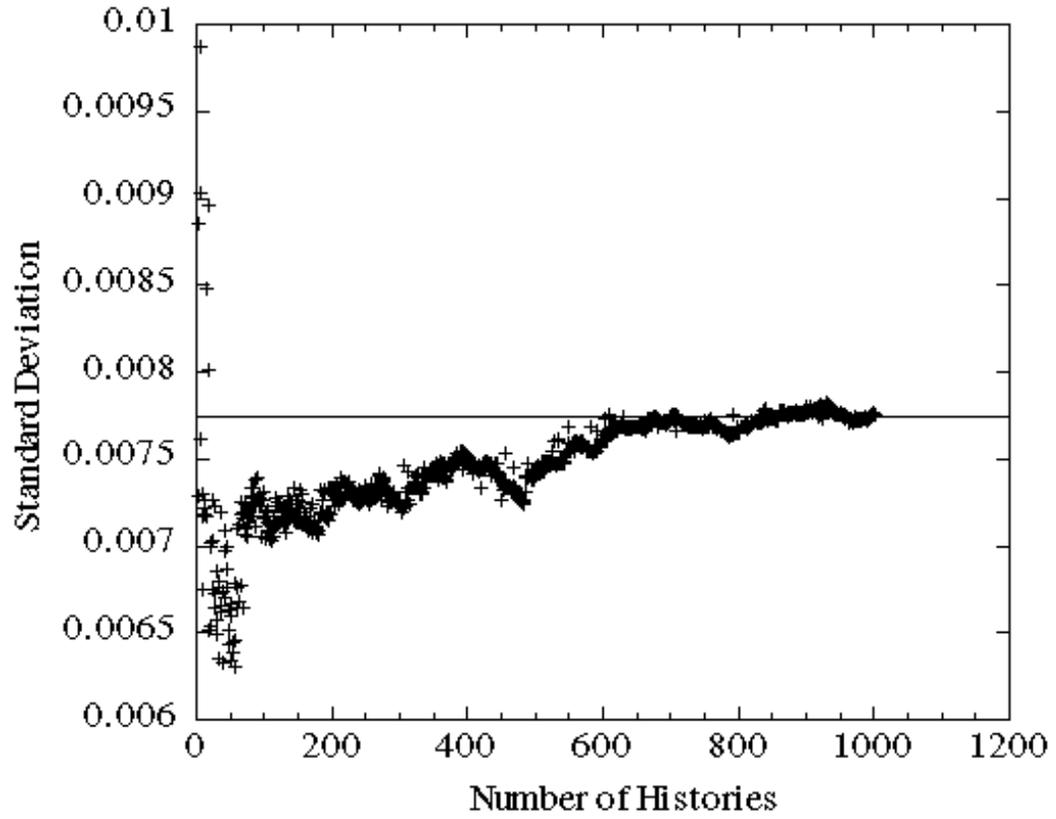


Figure 1. Convergence for KRONOS as a function of number of calculations.

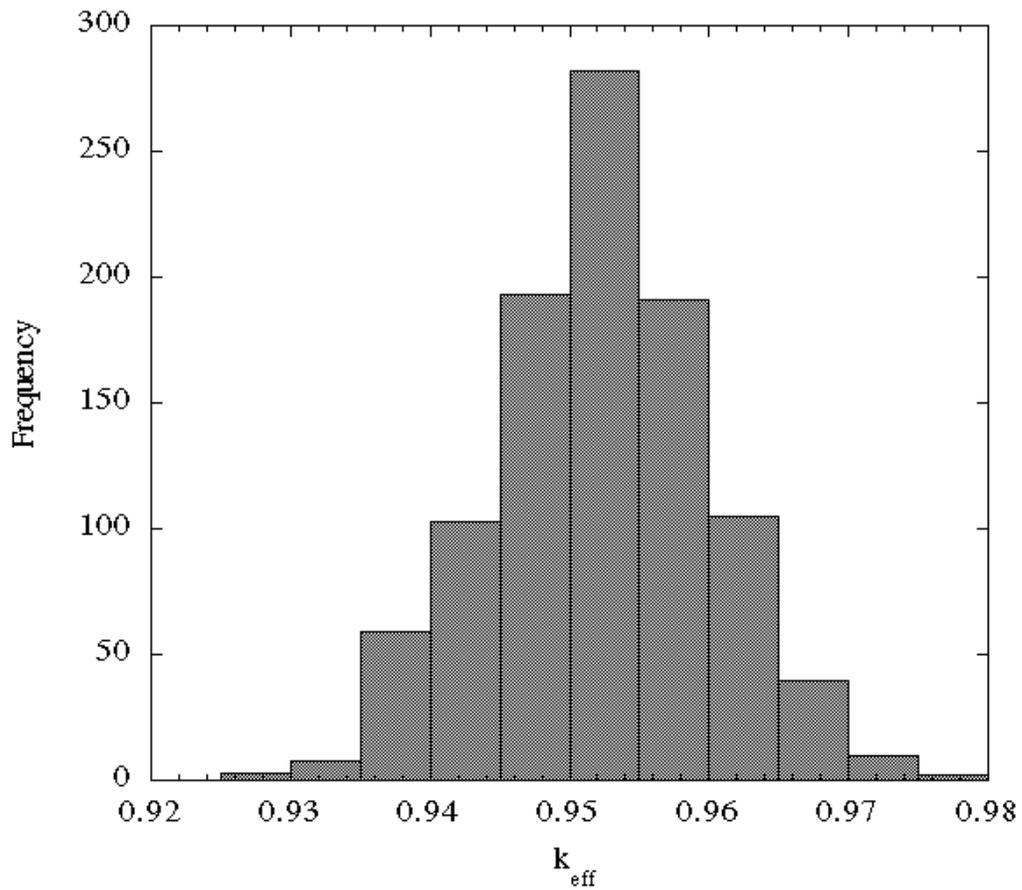


Figure 2. Histogram of KRONOS k_{eff} results for 1000 calculations.

Results

Calculations have been performed for both pin-cell and cask configurations, for several burnups, with uniform and axially varying burnup profiles, and both with and without fission products included in the evaluation. Table 1 lists the uncertainty (standard deviation) for a subset of these analyses.

Table 1. Standard Deviation of Variation in k_{eff} as Nuclide Inventories are Sampled Using
KRONOS

Fission Products Included?	Axial Burnup Profile?	Burnup (GWd/MTU)		
		20	40	60
Yes	Yes	0.0119	0.0169	0.0178
Yes	No (uniform)	0.0286	0.0292	0.0282
No	Yes	0.00412	0.00776	0.00817

As would be expected, the uncertainty is substantially larger when fission products are included, since, overall, uncertainties on fission products are larger than for actinides. Furthermore, the use of an explicit axial distribution reduces the uncertainty relative to a uniform burnup assumption, most likely due to the fact that the uniform burnup assumption overweights the importance of fission products. Finally, it is observed that the uncertainty increases with increasing burnup when an axial burnup distribution is used, but that it remains essentially constant with burnup when a uniform burnup profile is assumed. The reason for this is not so obvious, and will require further study.

Conclusions

A method has been developed to incorporate biases and uncertainties in isotopic predictions into an uncertainty term for neutron multiplication. Uncertainties derived in this manner can be applied in a conservative fashion without paying the penalties associated with the ultra-conservative method most commonly employed in proposed methodologies. This

approach requires further study, but may yield a better understanding of the effect of isotopic distributions and their uncertainties in burnup credit analyses. The approach is also CPU-intensive and design specific, but with further work may eventually allow a generalized assessment of the uncertainty in k predictions due to isotopic uncertainties.

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