

Using Cross-Section Uncertainty Data to Estimate Biases

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INTRODUCTION

Ideally, computational method validation is performed by modeling critical experiments that are very similar, neutronically, to the model used in the safety analysis. Similar, in this context, means that the neutron multiplication factors (k_{eff}) of the safety analysis model and critical experiment model are affected in the same way to the same degree by variations (or errors) in the same nuclear data. Where similarity is demonstrated, the computational bias calculated using the critical experiment model results is “applicable” to the safety analysis model. Unfortunately, criticality safety analysts occasionally find that the safety analysis models include some feature or material for which adequately similar well-defined critical experiments do not exist to support validation. For example, the analyst may want to take credit for the presence of fission products in spent nuclear fuel. In such cases, analysts sometimes rely on “expert judgment” to assign an additional administrative margin to compensate for the validation weakness or to conclude that the impact on the calculated bias and bias uncertainty is negligible.

Due to advances in computer programs and the evolution of cross-section uncertainty data, analysts can use the sensitivity and uncertainty analyses tools implemented in the SCALE TSUNAMI codes to estimate the potential impact on the application-specific bias and bias uncertainty resulting from nuclides that are under-represented or not present in the critical experiments. This paper discusses the method, computer codes, and data used to estimate the potential contribution toward the computational bias of individual nuclides. The results from application of the method to fission products in a burnup credit model are presented.

DESCRIPTION OF THE WORK

The SCALE 5.1 TSUNAMI-3D sequence uses flux moments calculated in forward and

adjoint KENO V.a calculations together with cross-section data and linear perturbation theory¹ to calculate the sensitivity of the system multiplication factor (e.g., k_{eff}) to minor perturbations in nuclear data. The sensitivities inherent in the resonance self-shielding calculations are also included. The sensitivity is calculated as relative sensitivity in units of $(\Delta k/k) / (\Delta\sigma/\sigma)$. The SCALE 238 neutron energy group ENDF/B-VI nuclear data library was used for the transport calculations.

The TSUNAMI-IP module can combine the sensitivity profiles for a model with the nuclear data uncertainty information distributed with SCALE in the form of covariance matrices. However, formally evaluated uncertainty data are not available for many important nuclides and reactions. In the SCALE uncertainty data files,² the evaluated data has been supplemented with approximate uncertainty data, yielding significantly more complete uncertainty data sets. The nature of the uncertainty data and plans for further development will be discussed in the presentation.

In support of Yucca Mountain Project (YMP) post-closure criticality safety,³ the SCALE 5.1 TSUNAMI-3D sequence was used to calculate the k_{eff} sensitivity profiles for a transportation, aging, and disposal (TAD) cask loaded with 21 B&W 15×15 fuel assemblies that had initial enrichments of 5 wt % ²³⁵U and were burned to 40 GWd/MTU. The TSUNAMI-IP module was then used to combine the model-specific energy-dependent sensitivity profiles with the energy-dependent cross-section uncertainty data contained in the 44 neutron energy group ENDF/B-VI “recommended” dataset (44groupv6rec) to produce model-specific k_{eff} uncertainty values for each nuclide and reaction occurring in the model.

RESULTS

The total one-standard-deviation uncertainty in k_{eff} resulting from the nuclear data uncertainties for all nuclides present in the TAD

model and nuclear reactions occurring in the transport calculation was 0.604 % $\Delta k/k$. Applying a 95% confidence level, one would expect the total computational bias due to nuclear data errors would be less than ± 1.2 % $\Delta k/k$. This value is consistent with computational biases typically seen for models involving mixed-oxide ($UO_2 + PuO_2$) fuel with isotopic compositions similar to commercial spent nuclear fuel. The accuracy of the k_{eff} uncertainty results rests on the assumption that the cross-section uncertainty data are reasonably accurate.

TABLE I. Model-Specific Nuclear Data Uncertainties for Fission Products

| Nuclide | % $\Delta k/k$ | Nuclide | % $\Delta k/k$ |
|-------------------|----------------|-------------------|----------------|
| ¹⁴³ Nd | 0.042 | ¹⁵³ Eu | 0.010 |
| ¹⁰³ Rh | 0.027 | ¹⁵² Sm | 0.009 |
| ¹⁴⁵ Nd | 0.023 | ¹⁵⁰ Sm | 0.006 |
| ¹⁴⁹ Sm | 0.022 | ⁹⁵ Mo | 0.005 |
| ¹⁰¹ Ru | 0.021 | ¹⁰⁹ Ag | 0.003 |
| ⁹⁹ Tc | 0.015 | ¹⁵⁵ Gd | 0.003 |
| ¹⁵¹ Sm | 0.014 | ¹⁵¹ Eu | 0.0004 |
| ¹⁴⁷ Sm | 0.011 | All FP | 0.069 |

The results for 15 fission products credited in the YMP analysis are presented in Table I. Fission products are primarily thermal neutron absorbers. The thermal neutron absorption cross sections are fairly smooth and the approximate uncertainty data is probably a good uncertainty estimate.

The total uncertainty due to the 15 modeled fission products may be obtained by taking the square root of the sum of the squares of the fission product uncertainty values in Table I and is 0.069 % $\Delta k/k$. At a 95% confidence level, it is expected that the total computational bias due to errors in the fission product nuclear data will be less than ± 0.14 % $\Delta k/k$. In the absence of suitable critical experiments with which to calculate a bias that includes bias due to fission products, it would be conservative to adopt a three-standard-deviation penalty of 0.21 % $\Delta k/k$ to account for the uncertainty in the reactivity of the fission products. Note that this analysis covers only the bias in calculated k_{eff} due to nuclear data errors and does not address a bias that may exist due to the methods used to calculate the spent fuel compositions. This technique is useful for estimating bounding

values for penalties to cover nuclear data biases for nuclides that cannot be properly validated with critical experiments.

REFERENCES

1. B. T. REARDEN, "SAMS: Sensitivity Analysis Module for SCALE," ORNL/TM-2005/39, Version 5.1, Vol. II, Book 4, Sect. F22, Oak Ridge National Laboratory (November 2006).
2. B. L. BROADHEAD, "SCALE 5.1 Cross-Section Covariance Libraries," ORNL/TM-2005/39, Version 5.1, Vol. I, Book 3, Sect. M19, Oak Ridge National Laboratory (November 2006).
3. G. RADULESCU, D. E. MUELLER, S. GOLUOGLU, D. F. HOLLENBACH, and P. B. FOX, "Range of Applicability and Bias Determination for Postclosure Criticality of Commercial Spent Nuclear Fuel," ORNL/TM-2007/127, Oak Ridge National Laboratory (October 2007).