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APPLICATION OF TSUNAMI AND TSURFER FOR VALIDATION OF BURNUP CREDIT IN THE CRITICALITY SAFETY ANALYSIS OF A TRANSPORT CASK

M. Behler
Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS) mbH, Forschungszentrum Boltzmannstr. 14, 85748 Garching near Munich, Germany

R. Kilger
Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS) mbH, Forschungszentrum Boltzmannstr. 14, 85748 Garching near Munich, Germany

M. Kirsch
Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS) mbH, Forschungszentrum Boltzmannstr. 14, 85748 Garching near Munich, Germany

M. Wagner
Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS) mbH, Forschungszentrum Boltzmannstr. 14, 85748 Garching near Munich, Germany

ABSTRACT

In up-to-date criticality safety analysis of spent nuclear, fuel modern calculation methods are applied to take into account the reduction of reactivity of nuclear fuel due to the burnup process. The use of these methods has to be validated by comparison to experimental data and usually this leads to a bias, which has to be considered in the neutron multiplication factor k_{eff}. Applying the so-called burnup credit, this task is complex since any fission products and actinides considered in the calculation have to be validated by adequate experiments. However, for typical applications like a spent fuel transport cask there are no public available experimental data which directly match the conditions of an application and include all the fission products typically being used. Thus the user is obliged to validate the fission products separately by choosing experimental data which match the conditions of the application at least partially and include one or more of the fission products of interest. Since 2009 new tools in the latest version 6 of the American code package SCALE ("Standardized Computer Analyses for Licensing Evaluation") from Oak Ridge National Laboratory have been provided to study and quantify the bias and uncertainty of an application calculation based on the validation calculations of experiments. E.g., a dedicated analysis tool named TSUNAMI can be used to quantify the similarity of an experiment to the respective application.

We are applying these tools, amongst those especially TSUNAMI and TSURFER, to a generic cask model and study their potential with regard to a possible validation. The experimental data used are taken from the International Criticality Safety Benchmark Evaluation Project (ICSBEP), an internationally supported benchmark database of high quality. TSURFER is intended to allow for the determination of the bias of a computation even if no experiment exactly matching the application condition is available. Special attention will be drawn to the influence of the fission products on the bias and the reliability of this bias in dependence on the available experiments.

INTRODUCTION

In modern calculation methods used in criticality safety analyses of nuclear spent fuel the reduced reactivity of the nuclear fuel due to the burnup process is taken into account. These methods have to be validated by comparing their results to experimental data and any deviation from the experimental data has to be considered as a computational bias to the neutron multiplication factor k_{eff} in the criticality safety analysis. The validation of the use of the so-called burnup credit, i.e. taking the reduced reactivity of the nuclear spent fuel into account, leads to a complex task since any fission products and actinides considered in the calculation have to be validated by adequate experimental data. Typically there are no public available experiments which match the conditions of a typical application as a spent fuel transport cask and which include all fission products being used. Thus, the consideration of each fission product can only be validated separately by using experimental data which match the conditions of the application at least partially and include one or more fission products of interest. For this purpose a dedicated analysis tool named TSUNAMI [1] was developed at Oak Ridge National Laboratory (ORNL) to quantify the similarity of experiments to the application. In the last version 6 of the code package SCALE [1] from ORNL new tools including TSURFER have been provided to study and quantify the bias and uncertainty of an application calculation based on validation calculations.

In this paper we are presenting the application of TSUNAMI and TSURFER to a generic transport cask model to study the potential of TSUNAMI and TSURFER in future validation processes.

TSUNAMI

Although modern neutron transport codes can predict k_{eff} with a high degree of precision, computational biases of a percent or more are often found when using these codes to model critical benchmark experiments. One primary source of this computational bias is believed to be errors in the cross-section data, as bounded by their uncertainties. A typical way to evaluate the computational biases and uncertainties of the computational methods and nuclear data is using a trending analysis, usually a linear regression with a statistical confidence band. For a traditional trending analysis, a suite of experimental benchmarks is selected with physical characteristics that are similar to the corresponding values in the application for which the neutron multiplication factor k_{eff} has to be calculated [2]. Each experiment is modeled with the same code and cross-section data that will be used for the application. The difference between the measured and calculated values of k_{eff} of a critical experiment is considered to be the computational bias for that experiment. The expected computational bias of the application is established through a trending analysis of the bias for all selected critical experiments as a function of their physical characteristics. The uncertainty in the bias is established through a statistical analysis of the trend, taking into account the uncertainty in each k_{eff} data point and the distribution of the data.

TSUNAMI provides a unique means of determining the similarity of nuclear criticality experiments to safety applications [3]. The basis is that computational biases are primarily caused by errors in the cross-section data, which are quantified in cross-section-covariance data. Instead of using average physical parameters to characterize a system, TSUNAMI determines the uncertainty shared between two systems, which directly relates to the bias shared by the two systems. To accomplish this, the sensitivity of k_{eff} to each groupwise nuclide-reaction specific cross section is computed for all systems considered in the analysis. Correlation coefficients are developed by propagating the uncertainties in neutron cross-section data to uncertainties in the computed neutron multiplication factor for experiments and application through sensitivity coefficients defined as $S_{k,\alpha} = \frac{\Delta k}{k}\frac{\alpha}{\Delta\alpha}$, where k is the neutron multiplications factor and α is a nuclear macroscopic cross section of a nuclide of interest. The bias in the experiments, as a function of correlated uncertainty with the intended application, is extrapolated to predict the bias and bias uncertainty in the target application.

TSURFER

The prediction of computational biases with the nuclear data adjustment tool TSURFER is based on a generalized linear least squares approach. TSURFER identifies a single set of adjustments to nuclear data that will result in the computational models all producing k_{eff} values close to their experimental k_{eff} value. This is done by minimizing chi-square, expressed as $\chi^2 = \Delta\alpha^T C_{\alpha\alpha}^{-1}\Delta\alpha + \Delta m^T C_{mm}^{-1}\Delta m$, where $\Delta\alpha$ and Δm describes the relative change in the nuclear data and in the measured response, respectively, and $C_{\alpha\alpha}^{-1}$ and C_{mm}^{-1} are the relative covariance matrices of the nuclear data and the experiments, respectively. Then the same data adjustments are used to predict an unbiased k_{eff} value for the application and an uncertainty in the adjusted k_{eff} value. The difference between the originally calculated k_{eff} value and the new postadjustment k_{eff} value represents the bias in the original calculation, and the uncertainty in the adjusted value represents the uncertainty in this bias. If similar experiments are available to validate the use of a particular nuclide in the application, the uncertainty of the bias for this nuclide is reduced. Experiments that are dissimilar from the application can still provide useful information for bias assessment if at least one material demonstrates similar sensitivities to those of the applications. Thus, with a complete set of experiments to validate important components in the application, a precise bias with a small uncertainty can be predicted. However, since TSURFER is based on a linear approximation for the propagation of data uncertainties, problems might appear in case of sizeable uncertainties where a linear approximation is not justified.

TSAR

The TSAR module in SCALE [1] performs sensitivity/uncertainty (S/U) calculations for responses represented by the *difference* of two eigenvalues. These types of responses are often of interest in reactor physics applications or in the analysis of critical experiments for nuclear data testing and validation studies. Data and methods deficiencies can introduce a computational bias manifested as a trend in calculated critical eigenvalues versus experiment parameters. TSAR can be applied to the *difference* in the computed eigenvalues of two benchmarks to establish the sensitivity of the bias trend to various nuclear data used in the calculations.

TSAR builds upon capabilities of other SCALE modules. The TSUNAMI-3D or -1D sequence is first used to calculate sensitivities for the multiplication factors of the reference and altered cases respectively. TSAR reads the sensitivity data produced by TSUNAMI k_{eff} calculations and uses them to compute relative or absolute sensitivities of an eigenvalue-difference response. TSAR also combines the calculated reactivity sensitivity coefficients with input nuclear data covariance matrices included in SCALE to determine the uncertainty of the reactivity response

APPLICATION

Application model

In the context of a generic criticality safety analysis, TSUNAMI and TSURFER were applied to a generic model of a spent fuel transport cask to estimate the computational bias of the criticality calculations. The model is taken from the Burnup Credit Criticality Benchmark phase II-C of the OECD/NEA Expert Group on Burnup Credit Criticality Safety [4].

The generic transport cask is simplified to a stainless steel cylinder (figure 1) which is completely flooded with pure water and contains 21 PWR 18x18-24 fuel assemblies in borated stainless steel baskets. The fuel assemblies consist of 300 fuel rods and 24 guide thimbles. The fuel rods are divided in 32 axial nodes. The fuel cladding and the guide thimbles are made of Zircaloy-4. Upper and lower assembly hardware is represented by regions of smeared stainless steel and water. A detailed geometrical description can be found in the benchmark report [4].

For the study presented here, the cask is filled with 21 identical fuel assemblies with an initial enrichment of 4.0% ^{235}U and an average burnup of 40 GWd/t_{HM}. The spent fuel nuclide inventories were calculated using the depletion code OREST, Version 2006 [5], developed at GRS. A cooling time of 5 years were taken into account and the actinides ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu,

^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am and ^{243}Am, the fission products ^{109}Ag, ^{133}Cs, ^{151}Eu, ^{153}Eu, ^{155}Gd, ^{95}Mo, ^{143}Nd, ^{145}Nd, ^{103}Rh, ^{101}Ru, ^{147}Sm, ^{149}Sm, ^{150}Sm, ^{151}Sm, ^{152}Sm and ^{99}Tc, and ^{16}O were considered. Performing a best estimate criticality calculation leads to a neutron multiplication factor of k_{eff} = 0.84743 ± 0.00021 while a conservative criticality calculation taking into account bounding conditions in geometry, enrichment, burnup profile, depletion calculation, neglecting single fission products due to lack of validation data, etc. results in a multiplication factor of k_{eff} = 0.93833 ± 0.00017 [6].

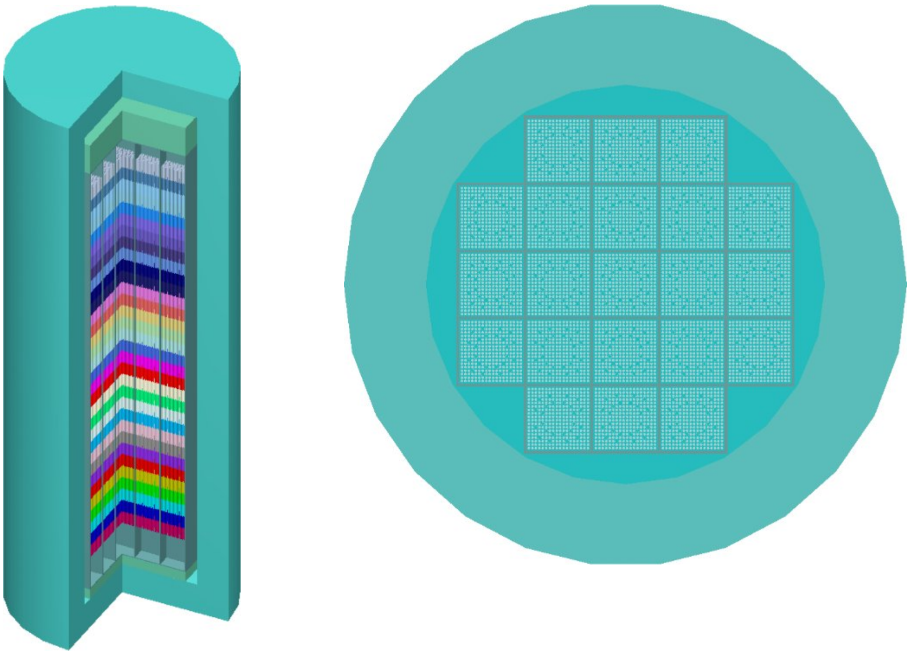

Figure 1. KENO V.a model of the generic transport cask with 21 PWR fuel assemblies. The fuel assemblies are divided in 32 axial nodes.

Experimental data

The experimental data to validate the criticality calculations were taken from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) [7]. A total of 31 experiments from 6 different series were modeled in detail and analyzed using TSUNAMI (table 1).

Table 1. List of experiments used in the validation analysis.

No.	Experimental series	cases
1	leu-comp-therm-003	3
2	leu-comp-therm-050	9
3-14	leu-misc-therm-005	1 - 12
15-20	leu-comp-therm-052	1 - 6
21-26	mix-comp-therm-008	1 - 6
27-31	mix-comp-therm-007	1 - 5

The sensitivity analysis were performed with the corresponding sequence TSUNAMI-3D-K5 from the SCALE 6.0 code package using the nuclear cross section library ENDF/B-VII in 238 energy group and modules KENO-V.a for the neutron transport calculation and CENTRM for the resonance treatment.

A proper adjustment of the nuclear cross sections using TSURFER requires the knowledge of possible correlations between experimental uncertainties of different experiments. This is of particular importance in the case of experimental series where strong correlations can be expected. Often, such correlations are not given in the experiment descriptions and the user has to estimate the correlations by analyzing the experimental setups. Our assumptions are shown in figure 2.

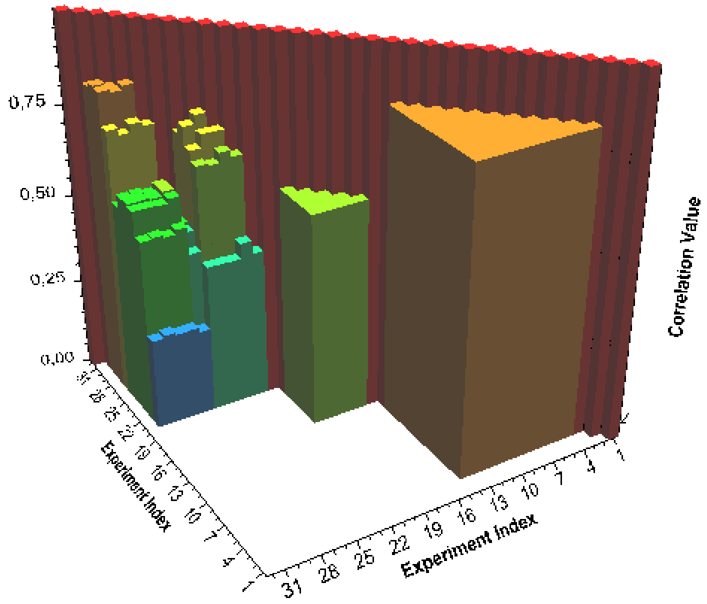

Figure 2. Correlation matrix of the experiments.

TSURFER performs a test on the calculated χ^2 to detect potential inconsistencies in the experimental date which are indicated by a large χ^2. Such inconsistencies could be due to underestimated uncertainties or erroneous assumptions for the correlations in the experimental or nuclear data, or due to underestimated simplifications in the computational models. In the case the χ^2 exceeds a certain value, TSURFER excludes the experiment with the largest impact on χ^2 and repeats the calculation. In case of the experimental data listed in table 1 and using the standard configuration TSURFER omits six experiments: leu-comp-therm-003 case 3, leu-comp-therm-050 case 9, leu-misc-therm-005 case 1 and 9, and leu-comp-therm-052 case 1 and 3.

Using one experiment as an application and comparing the calculated bias from TSURFER with the difference between simulated and measured k_{eff} could give additional hints on potential inconsistencies. Table 2 gives some examples, which showing incompatible multiplication factors for the first two omitted experiments and well compatible results for the other three examples, even if the third one is also omitted. For the further studies we restricted the experimental data to the list of experiments accepted by TSURFER.

Table 2. Bias estimated by TSURFER for different experiments.

Experiment	K_{eff}, calc.	K_{eff}, exp.	Bias, exp.	Bias, TSURFER
leu-comp-therm-003/3	0.9882(2)	1.0000±0.0039	-0.0118±0.0039	+0.0001±0.0010
leu-comp-therm-050/9	0.9966(2)	1.0000±0.0010	-0.0034±0.0010	+0.0020±0.0013
leu-misc-therm-005/3	1.0028(2)	0.9999±0.0007	+0.0029±0.0007	+0.0025±0.0006

leu-misc-therm-005/11	1.0027(2)	0.9998±0.0007	+0.0029±0.0006	+0.0023±0.0006
mix-comp-therm-008/1	0.9975(1)	0.9997±0.0031	-0.0022±0.0031	-0.0030±0.0026

RESULTS

The analysis performed by TSURFER results in a computational bias of Δk_{eff} = -0.00230 ± 0.00213. The main contributions to this bias are listed in table 3.

Table 3. Main Contributions to the computational bias estimated using standard conditions (absolute numbers).

Nuclide	Reaction	Contribution to bias	Nuclide	Reaction	Contribution to bias
^{239}Pu	nubar	- 0.00092	^{90}Zr	elastic	0.00018
^{235}U	nubar	- 0.00062	^{1}H	elastic	0.00017
^{238}U	n,gamma	- 0.00048	^{235}U	chi	- 0.00012
^{235}U	fission	- 0.00032	^{235}U	n,gamma	- 0.00018
^{239}Pu	fission	- 0.00027	^{238}U	nubar	- 0.00016
^{238}U	n,n'	0.00022	^{149}Sm	n,gamma	0.00013
^{133}Cs	n,gamma	0.00019	^{238}U	elastic	- 0.00009

Effect of correlations and underestimated uncertainties

The exclusion of certain experiments in general points to either a problem with the calculation or a problem with the experiment. Assuming the calculation model is correct, it might be interesting to study the impact of correlations and potentially underestimated uncertainties on the bias.

For the experiments in the ICSBEP simplified computational models and corresponding corrections to the multiplication factors estimated from simulations are proposed but typically no additional uncertainties due to the use of simulations are applied. For experimental series with small experimental uncertainties like leu-comp-therm-050 and leu-misc-therm-005, this could lead to an underestimation of the total uncertainty. We increased the uncertainties of these experimental series to δk_{eff} = 0.0015 instead δk_{eff} = 0.0010 (leu-comp-therm-050) and δk_{eff} = 0.0007 (leu-misc-therm-005) to study a potential impact on the bias. In this case only two experiments (leu-comp-therm-052 case 1 and 3) are omitted by TSURFER and the bias is estimated to Δk_{eff} = -0.00184 ± 0.00211. The main contributions to the bias are listed in table 4.

Different sets of correlations were also analyzed. For example, in the case of neglecting the correlations five experiments were omitted (leu-comp-therm-050 case 9 and leu-comp-therm-052 case 1, 2, 5 and 6) and a bias of Δk_{eff} = -0.00153 ± 0.00200 was estimated. The main contributions are listed in table 4.

Table 4. Main Contributions to the computational bias estimated using increased experimental uncertainties.

Increased uncertainty			No correlations		
Nuclide	Reaction	Contribution to bias	Nuclide	Reaction	Contribution to bias
^{238}U	n,gamma	- 0.00113	^{238}U	n,gamma	- 0.00178
^{235}U	nubar	- 0.00067	^{238}U	n,n'	- 0.00029
^{235}U	fission	- 0.00027	^{238}U	nubar	- 0.00028
^{90}Zr	elastic	0.00026	^{90}Zr	elastic	0.00026

^{235}U	n,gamma	- 0.00019	^{235}U	chi	- 0.00015
^{149}Sm	n,gamma	0.00018	^{1}H	elastic	0.00021
^{238}U	nubar	- 0.00016	^{239}Pu	fission	- 0.00017

The comparison of table 3 and 4 shows large differences in the contributions and therefore large differences in the adjustment of the nuclear data for the discussed cases, even if the bias changes only moderately. It demonstrates the sensitivity of the adjustment on the data set used.

Partial bias of fission products

TSURFER already provides the single contributions to the bias (table 3) and thus the partial bias of a fission product of interest can be extracted form this table. Due to the small sensitivity $S_{\alpha,k}$ of the fission products this approach should lead to large relative uncertainties in the partial bias.
In case of an experimental series containing similar experiments which differ only in the content of one fission product, like leu-misc-therm-005 case 3-6, TSAR provides the possibility to analyze the difference of two experiments. The reactivity-difference response is dominated by the fission product, ^{133}Cs in the case of leu-misc-therm-005 case 3-6, and therefore the fission product shows the largest sensitivity to reactivity-difference response.

A more sophisticated approach is proposed in [8]. A set of experiments without fission products and one difference between a reference case and a case with an additional fission product is used. Applying TSURFER to the fission product experiment as the “application” provides the partial bias due to the fission product for this particular experiment. Repeating this for several experiments, correcting the results with the ratios of sensitivities and neutron multiplications factors of the experiment and the real application, adding a penalty factor to take dissimilarities between experiment and real application into account and averaging the results leads to the partial bias of the fission product for the application.
We applied this approach to the experiments leu-misc-therm-005 case 3-6 to determine the partial bias of ^{133}Cs but neglecting the penalty for a first study and used the case 3 as the reference case.

Table 5. Partial bias of ^{133}Cs determined for experiments leu-misc-therm case 3-6.

Experiment	Exp. partial bias	Sensitivity $S_{k,\alpha}$	$\hat{g}$	App. partial bias
leu-misc-therm-005 / 4	0.000001	-1.0735E-05	0.8041	0.000004
leu-misc-therm-005 / 5	0.000074	-3.0102E-05	0.8086	0.000115
leu-misc-therm-005 / 6	0.000200	-6.5338E-05	0.8130	0.000143

The application biases extracted from each experiment show large variations which lead to the conclusion that either a large uncertainty has to be assumed or the neglected penalty factor could provide a major contribution to the partial bias. This behavior is also shown in [8] but without any detailed discussion.

CONCLUSION

With TSUNAMI and TSURFER, the SCALE package provides powerful tools to estimate the computational bias. We applied both tools to a generic transport cask and studied their potential to provide useful information for validation of criticality safety calculations.

As discussed above, several details could influence the calculated bias. These are the correlations of uncertainties and also the uncertainties itself, which have been determined with models itself. The omission of experimental data, which have been judged to be potentially inconsistent by TSURFER, leads to a possible source of uncertainty since the impact on the χ^2 does not necessarily have to be correlated with a problem in the experimental data. This approach does not assure the omission of problematic experiments only. Hence the user should carefully examine all experiments to identify potential sources of inconsistencies and remove or correct the affected experimental data based on substantiated physical reasons. The main problem here is that TSURFER attributes all deviations between experiment and calculation to nuclear data, which however is not the case. Thus, deviations resulting from other sources as model assumption or resonance treatment end up in a data adjustment. In order to get reliable results it is important that the nuclear data provides the dominant contribution to the error.

The estimate of the partial bias of a single fission product was analyzed. The partial biases of the fission products are usually at least an order of magnitude smaller than the dominating biases of the fissile materials and show large variations suggesting large relative uncertainties. Furthermore comparing the partial bias of the fission products with biases typically introduced in criticality safety analyses due to conservative assumptions of $\Delta k \approx 0.1$ discussed above, a conservative assumption on the bias from fission products might be acceptable.

ACKNOWLEDGMENTS

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