Proceedings of the 18th International Symposium on the Packaging and Transportation of Radioactive Materials
PATRAM 2019
August 4-9, 2019, New Orleans, LA, USA

CRITICALITY CODES BIASES AND ASSOCIATED UNCERTAINTIES DETERMINATION FOR FISSILE NUCLEAR MATERIAL TRANSPORTATION USING DIFFERENT APPROACHES

Marcel TARDY
Orano TN, France
marcel.tardy@orano.group

Stavros KITSOS
Orano TN, France
stavros.kitsos@orano.group

David LIN
Orano TN, France
david.lin@orano.group

Laurent MILET
Orano TN, France
laurent.milet@orano.group

Stéphane NALLET
Orano TN, France
laurent.milet@orano.group

Nicolas LECLAIRE
IRSN, France
nicolas.leclaire@irsn.fr

Isabelle DUHAMEL
IRSN, France
isabelle.duhamel@irsn.fr

ABSTRACT

Criticality safety analysis regarding fissile nuclear material transportation or operations requires, among many aspects, the experimental validation of the criticality codes with the associated cross-section libraries. The requirements for the experimental validation of the criticality code is to analyze the similarity between a selected set of critical experiments and the industrial configuration studied to determine the calculational biases and the associated uncertainties using different methods.

The method currently used in France for addressing the bias and its associated uncertainty is mainly based on expert judgment and the knowledge of available experiments. This approach uses descriptive parameters (geometry, composition…) and some macroscopic calculated parameters to infer experiments potentially representative of an industrial case and the corresponding biases. The biases of the reference experiments are then transposed to the industrial case depending of the representativity of the experiments. This step can be facilitated by doing a linear regression of k_{eff} versus the parameter that best describes the configuration.

An alternative method is to study the similarity between the selected experiments and the industrial case using the statistical approach based on the Generalized Linear Least Square Method (GLLSM). This method allows the propagation of uncertainties in nuclear data and discrepancies between calculations and reference benchmarks for a selection of experiments to linearly adjust the calculated k_{eff} values to reference values and therefore exhibit a bias and uncertainty due to nuclear data for an industrial case.

The aim of the paper is to compare these two methodologies on an Orano TN transport and storage cask for BWR used fuel at around 15 GWD/MTU. A first selection of experiments was drawn using expert judgment. This selection was then restricted to experiments that were shown to be the closest to the industrial case regarding the C_k "similarity" parameter calculated with the SCALE 6.2.1 package. Applying both methodologies to the industrial case highlights that they both give comparable biases with regards to the uncertainties.

1 INTRODUCTION

Criticality analysis for a transport and storage cask containing used fuel assemblies requires the validation of the criticality codes and the associated cross-section libraries. The validation of criticality codes and the associated nuclear data can be divided into four steps:

– Step 1: the definition of the range of applicability based on the key parameters of the cask, such as moderator to fuel ratio, fissile isotope enrichment, reflector conditions, presence of neutron absorbers, etc.

– Step 2: the selection of a set of critical experiments similar to the cask configuration which can be done by identifying the main neutron-physical parameters having the most influence for the cask and the selected critical experiments.

– Step 3: the modeling of the critical experiments and the calculation of the k_{eff} values of the selected benchmark experiments.

– Final step: the analysis of the results in order to evaluate the computational bias and uncertainty associated with the industrial case.

A set of 361 experiments were selected for the criticality code validation used on an Orano TN transport and storage cask for BWR UO_2 used fuel assemblies.

This paper examines the two approaches used to compare the similarity between the selected experiments and the industrial case and to determine the calculational bias and uncertainty associated with nuclear data for the definition of the k_{eff} acceptance criterion for the criticality assessment.

The first approach, expert judgment, commonly used in France for criticality-safety assessment, is based on the identification of main global neutron-physical parameters having the most influence on the cask and the selected critical experiments. The second approach is based on sensitivity and uncertainty (S/U) analysis using the General Linear Least Squares Methodology (GLLSM [1]).

2 COMPUTATIONAL MODELS

2.1 Fuel assembly description

The fuel used for the study was a BWR UO_2 assembly design which consists of a 10×10 lattice and in which eight fuel rods were replaced with two large water rods as shown in Figure 1. The BWR UO_2 fuel assembly studied is highly heterogeneous with a maximum average enrichment of about 4.6 wt. % ^{235}U. It consists of a maximum of 92 fuel rods of varying ^{235}U enrichment (from ~2 wt. % up to ~5 wt. %) with UO_2 pure rods and with gadolinium added as burnable poison in some fuel rods. The assembly design also contains an outer zircaloy channel. It has a non-uniform axial loading, composed of a main central fuel region with non-uniform enrichment and gadolinium loading. In addition, axially “vanished” regions of the assembly resulting from the presence of partial-length rods are part of the assembly.

Sensitivity calculations [2] show that the use of a simplified model based on a uniform radial enrichment distribution with the maximum average enrichment of the assemblies, including the gadolinium fuel rods and a homogeneous axial lattice over the entire length of the assembly, is conservative from a criticality analysis point of view.

A cross-section view of the main axial zone of the assembly is illustrated in Figure 1.

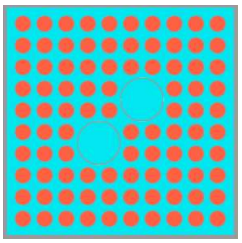

Figure 1 Cross-section view of the BWR UO_2 fuel assembly studied

2.2 Transport cask model

The cask used for transportation configuration calculations is the TN® 24 BH cask, which is an Orano TN representative transport and dry storage cask (see Figure 2 and Figure 3). In the configuration studied, it can be loaded with 65 BWR UO_2 nuclear used fuel assemblies that are separated by aluminum borated plates. The cask, the basket and the assemblies are modeled conservatively by taking into account the design parameters with their associated maximum or minimum bounding tolerances. Free spaces in the package are filled with full density water to cover the loading and unloading phases.

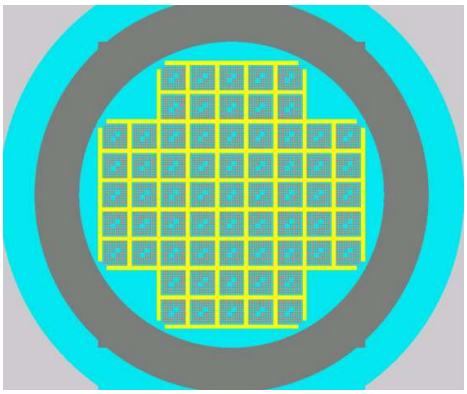

Figure 2 Cross section of BWR UO_2 assemblies in the TN 24® BH cask

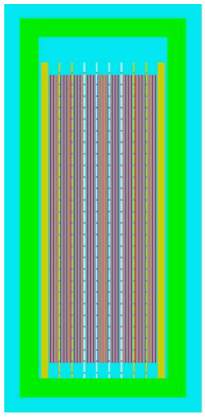

Figure 3 Axial view of BWR UO_2 assemblies in the TN 24® BH cask

3 METHODS, COMPUTER CODES AND NUCLEAR DATA

3.1 Methods

Two major methodologies were tested for assessing the bias associated with an Orano TN transport and storage cask configuration. The first one is based on expert judgment and is commonly used in the French criticality-safety practice. The second one uses the sensitivity/uncertainty techniques and reference k_{eff} to derive a bias for the Orano TN industrial configuration.

3.1.1 Expert judgment method

The expert judgment method consists, first, of the identification and the analysis of key neutron-physical parameters (e.g. enrichment, energy corresponding to average lethargy of neutrons causing fission (EALF), moderator to fuel ratio, geometrical arrangement, etc.) having the most influence for assessing the similarity between the industrial case and the selected critical experiments. The determination of bias and uncertainty can be done by calculating the C-E value for the selected experiments given by the calculated K_{eff} value of the critical benchmark experiments minus the benchmark k_{eff}, the dispersion of the population, the maximum and minimum values.

3.1.2 GLLSM methodology

The General Linear Least Squares Methodology (GLLSM [1]) is based on a data assimilation technique. The nuclear data uncertainties are propagated on the industrial case. The knowledge of experiments brings additional information that helps reduce the uncertainty on nuclear data that can reach 2000 pcm to 3000 pcm for some isotopes. In this approach, the discrepancies calculation/benchmark are assumed to be only due to nuclear data. Verification should ensure that there is no bias due to the calculation scheme.

3.1.2.1 Prior uncertainty

Nuclear data are by essence uncertain due to uncertainties in the measurement of cross sections, angular distributions, but also to the physical models used to match the experimental measurements. This uncertainty is intrinsic to nuclear data. Such information is contained in the covariance matrices provided with the evaluations.

Using sensitivity calculations, a prior uncertainty can be assessed on the k_{eff} due to nuclear data. The prior uncertainty is given by formula (1) and uses covariance data from nuclear data libraries.

$$\textbf{Prior Uncertainty} = \delta K_{prior} = \sqrt{S_k^{\,t} \times W^0 \times S_k} \quad (1)$$

S_k being the sensitivity vector of the industrial case and W^0 the nuclear data covariance matrix.

3.1.2.2 Posterior uncertainty

The knowledge of experiments close to the industrial case helps to decrease the uncertainty associated with nuclear data through the assimilation process.

A posterior uncertainty was evaluated using reference benchmark experiments and the GLLSM methodology [1]. Taking into account the uncertainty associated with nuclear data, the uncertainty of selected experimental cases, the experimental and calculated k_{eff}, the nuclear data was adjusted so that the calculated and experimental k_{eff} coincide.

This assimilation of data was then applied to the industrial case using the TSURFER sequence of the SCALE 6.2.1 package [3]: the bias as stated in formula (2) was obtained by multiplying the variation of nuclear data by the sensitivity of k_{eff} to these cross sections.

The uncertainty is calculated after adjustment of the covariance matrix (W^1) given in formula (2) where W^1 is the posterior covariance matrix, S is the sensitivity to nuclear data matrix, and S^T is its transpose, and where W^0 is the prior covariance matrix and C is the experimental covariance matrix.

$$W^1 = \left(W^{0^{-1}} + [S^T C^{-1} S]\right)^{-1} \quad (2)$$

3.1.2.3 Determination of bias

The bias was calculated by formula (3), using sensitivity coefficients and the posterior covariance matrix, as well as the k_{eff} discrepancies (Δk_{eff}) observed on the selection of representative benchmarks.

$$\text{Bias} = S \times \Delta\sigma = S \times [W^1 S^T C^{-1} \Delta k_{eff}] \quad (3)$$

W^1 is the covariance matrix after adjustment of cross sections with benchmark experiments.

3.2 Codes and nuclear data

All transport k_{eff} calculations were carried out using the SCALE 6.2.1 package associated with the continuous energy KENO-V.a code and the ENDF/B-VII.1 nuclear data library.

Sensitivity calculations were carried out using the TSUNAMI-3D sequence of the SCALE 6.2.1 package [3].

To address the similarity between the benchmarks and the Orano TN configuration, the TSUNAMI-IP sequence [4] of the SCALE 6.2.1 package was used.

Finally, the calculational bias was assessed using the GLLSM methodology implemented in the TSURFER sequence [1] of the SCALE 6.2.1 package.

4 ANALYSIS OF INDUSTRIAL CONFIGURATIONS

Two configurations involving the TN® 24 BH transport cask loaded with 65 BWR UO_2 used fuel assemblies were studied. The burnup of the used fuel assemblies loaded in the cask lies in general between 10-15 GWd/MTU, which corresponds to the burnup range of the consumption of nearly all of the gadolinium content in the fuel assemblies (gadolinium peak reactivity). For both configurations, the conservative approach used for criticality safety analysis considered main actinides exclusively (^{235}U, ^{236}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{242}Pu), and the residual gadolinium at the peak reactivity resulting from the depletion of the BWR UO_2 fuel was neglected. The key parameters of both configurations are given in Table 1.

Table 1 Parameters for industrial cases

TN®24 BH configuration	k_{eff} +/-σ	Average enrichment (wt. %)	Pu/(U+Pu) (wt. %)	EALF	V_{mod}/V_{ox}
Case 1	0.93140 +/- 0.00030	3.322	0.548	0.437	3.000
Case 2	0.93470 +/- 0.00032	3.478	0.453	0.356	3.198

TSUNAMI-3D calculations were carried out with KENO-V, a continuous energy code of the SCALE 6.2.1 package and the ENDF/B-VII.1 associated library to determine the neutronic characteristics of both industrial configurations precisely. Indeed, the reactions having the greatest impact on the cask reactivity were determined with the obtained sensitivity coefficients for these calculations. The list of main contributors to the sensitivity of the cask k_{eff} is given in Table 2.

Table 2 List of main contributors to the sensitivity of k_{eff}

Reaction	Location	Integral sensitivity of k_{eff}	
		Case 1	Case 2
^{235}U, nubar	Fuel assembly	0.706	0.752
^{235}U, fission		0.264	0.263
^{239}Pu, nubar		0.214	0.163
^{239}Pu, fission		0.100	0.093
^{238}U, capture		-0.149	-0.123
^{238}U, fission		0.041	0.036
^{10}B, capture (n,a)	Basket	-0.052	-0.051
^{27}Al, capture		-0.0088	-0.0090
^{56}Fe, capture	Basket + Cask	-0.0078	-0.0079

It can be pointed out that the main reactions of interest are the fission of ^{235}U, ^{238}U, ^{239}Pu, nubar of ^{239}Pu and ^{235}U, and the capture of ^{56}Fe, ^{27}Al, ^{238}U and ^{10}B. A comparison of sensitivity profiles for the main reactions shows that the two industrial configurations studied are quite similar. Figure 4 gives a comparison of the sensitivity profiles of k_{eff} to ^{235}U fission for both industrial configurations studied.

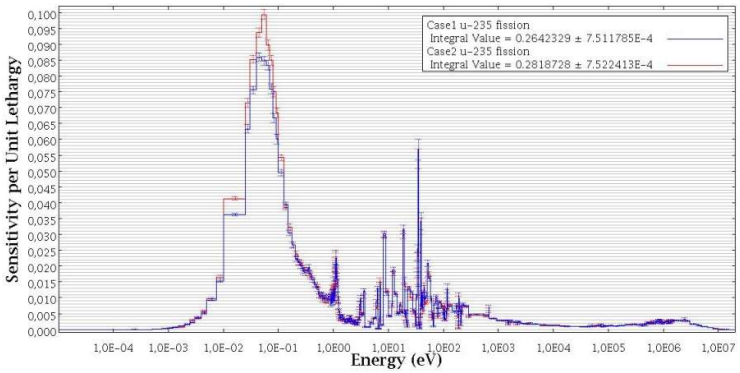

Figure 4 Sensitivity profile of k_{eff} to ^{235}U fission

5 PRELIMINARY SELECTION OF REPRESENTATIVE EXPERIMENTS

5.1 Selection method

The selection of experiments was first based on expert judgment to identify the benchmarks that were assumed to be closest to the Orano TN transport & storage cask configuration. The parameters used in such an approach were the chemical characteristics of the industrial case as well as its geometry. The benchmarks were mostly extracted from the ICSBEP Handbook [5], which describes the experiments following a standard format, and which also provides the propagated uncertainties and a benchmark model that can be easily modeled by most transport codes. Special attention was paid to selecting a sufficient number of benchmarks coming from various laboratories for statistical purposes which exhibited low experimental uncertainties and in order to have low correlated experiments.

The sensitivity coefficients of the Orano TN cases and the sensitivity profiles of selected benchmarks were compared so as to confirm the validity of the selection.

Moreover, no limitation was placed on the selection in order to have a sufficiently large number of experiments that could "surround" the industrial case. It was verified "*a posteriori"* that the experiments were sufficiently close to the industrial configuration through similarity calculations using the TSUNAMI-IP [1] sequence of the SCALE 6.2.1 package [3].

5.2 Selected experiments

Configurations involving lattices of UO_2 and UO_2-PuO_2 rods in water, with or without aluminum canisters and with or without stainless steel or iron as a reflector, were selected.

As the industrial assemblies were poorly burned and, therefore, assumed to be close to UO_2 fresh fuel, lattices with UO_2 fuel with an enrichment of uranium lower than 10% of ^{235}U were mostly selected. However, to take into account the small burnup of the assemblies, French proprietary experiments involving high Burn-up[6]) rods (HTC - Haut Taux de Combustion), containing 1.1 % PuO2, and a mix of both UO_2 and high Burn-up rods (MIX-COMP-THERM-PF003 and MIX-COMP-THERM-PF005) conducted within the framework of the Fission Products program [7], were also selected.

As seen above, the industrial cases being quite sensitive to ^{56}Fe and ^{10}B, experiments involving separating materials with boron or iron or with borated water were added to the selection.

In order to study the influence of the moderation ratio on the bias, experiments with tight-packed lattices of rods were added to the selection (LEU-COMP-THERM-071 and LEU-COMP-THERM-073). To address the over-moderation created by the water rods at the center of the assembly, experiments with water layers, water holes or water crosses were also considered (LEU-COMP-THERM-073, LEU-COMP-THERM-039 and LEU-COMP-THERM-096).

Moreover, configurations representative of a transport cask (with absorbing canisters and steel reflectors), such as LEU-COMP-THERM-034 and LEU-COMP-THERM-040, were also kept. In addition, in order to validate the calculation of the aluminum separating assemblies and the iron reflector shell, experiments with structural materials were used.

In sum, 361 experiments were selected among which 308 were found to be consistent, the others being removed from the selection. A C_k calculation was conducted on this selection of 308 experiments and only the 40 most representative with regards to this parameter are gathered in Table 3.

Table 3 Most representative selected benchmark experiments for expert judgment methodology.

SERIES	Number of cases	^{235}U wt. %	Water hole/Water gaps	Reflector	Separator/ canister	Soluble absorber	Uncertainty (pcm)
LCT-005	1	4.31					660
LCT-008	16	2.46	Holes			Boron: 779 to 1384 ppm	120
LCT-011	4	2.46	Water gap		B_4C pins	Boron: 0 to 1037 ppm	180 to 320
LCT-014	1	4.31				Boron: 0 and 2.55 g/l	190 and 690
LCT-017	4	2.35		Depleted Uranium (7.65 cm thick), lead (10.2 cm) or Steel (17.85 cm thick)			280 to 310
LCT-042	1	2.35		Steel (17.85 cm thick)	Cadmium (0.61 mm) Steel (3.02 mm) Borated steel (2.98 mm) Boroflex (5.46 mm)		160 to 330

SERIES	Number of cases	^{235}U wt. %	Water hole/Water gaps	Reflector	Separator/ canister	Soluble absorber	Uncertainty (pcm)
					Copper-cadmium(3.57 mm)		
LCT-051	4	2.46			SS and Al/B Separators	15 to 514 ppm	190 to 240
LCT-055	2	3		Stainless steel (2.67 cm)			250
LCT-076	5	3	Water holes		Aluminium and Borosilicate rods		250
MCT-HTC-002	1	1.57% ^{235}U/1.1%Pu				Borated water (0.1 to 0.595 g/l)	247
MCT-HTC-004	1	1.57% ^{235}U/1.1%Pu		Lead	Cadmium		90 to 470

6 BIAS AND UNCERTAINTY

6.1 Expert judgment

The extended selection of 361 experiments described previously was first used to derive the bias associated with the Orano TN configuration.

Even if a good agreement was obtained for most series, the C-E observed for the selection of experiments using SCALE 6.2 and ENDF/B-VII.1 lies between 2165 pcm (LCT-057.c33) and -1261 pcm (LCT-012.c03) with an average C-E of -104 pcm and an associated dispersion of 345 pcm. For some series, tendencies to overestimate k_{eff} (LCT-057 for most cases) or to underestimate k_{eff} (LCT-012, LCT-051 and LCT-052 for some cases) were identified.

When analyzing the k_{eff} results in detail, the LCT-012 series seemed to be inconsistent with other similar series involving the same materials. As other codes gave the same trends, an experimental bias cannot be excluded; therefore, they were removed from the initial selection. Similarly, LCT-057 results, which calculate high for all codes and nuclear data libraries when compared with other LCT cases, were also removed from the selection of experiments. Once again, an experimental bias cannot be excluded. The same observation applies for LCT-052 (cases 1, 2, 5 and 6) and LCT-051 (cases 13, 14 and 18).

Considering the 308 remaining C-E values, the C-E values observed for the selection of experiments lay between 683 pcm (LCT-005.c12) and -621 pcm (LCT-051.c16), the experimental uncertainties varying between 50 pcm and 690 pcm. Finally, not to give too much weight to experiments that are highly correlated, only the averaged C-E of each series were considered in the calculation of the average between series.

The averaged C-E was therefore -13 pcm and the associated standard deviation was 208 pcm.

6.2 Analysis of Sensitivity/Uncertainty (S/U) and determination of bias

6.2.1 Uncertainty due to nuclear data

The first step in determining the bias in the nuclear data consisted of assessing the prior uncertainty in the nuclear data. It accounted for the nuclear data uncertainty despite the existence of benchmark experiments that contributed to an uncertainty reduction.

The prior uncertainty for both Orano TN cases is around 440 pcm, with the covariance data from the ENDF/B-VII.1 library.

As expected, the fission and nubar cross sections of ^{235}U, ^{239}Pu and the (n,γ) capture cross section of ^{238}U and ^{235}U were the main contributors to the uncertainty. In spite of its high contribution in terms of sensitivity to k_{eff}, boron is not identified as being a main contributor.

Moreover, as the uncertainties pertaining to the cross sections of ^{56}Fe are quite high (see Figure 2), even if the sensitivity of k_{eff} to the cross sections of ^{56}Fe is not so high (Table 2), iron appears to be a main contributor since the contribution of the ^{56}Fe cross sections to the uncertainty is high.

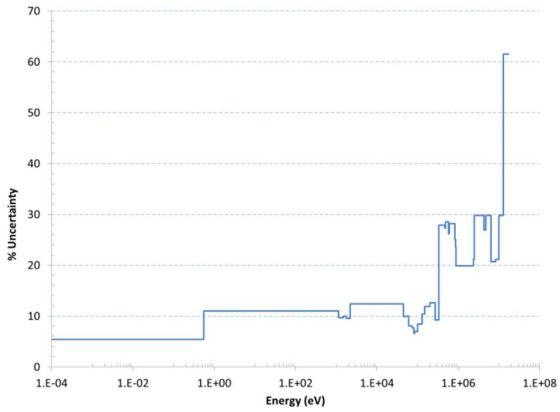

Figure 5 Uncertainty of ^{56}Fe capture cross sections – ENDF/B-VII.1 library

6.2.2 Determination of the C_k parameter

The benchmarks with the highest C_k values from the selection of the 361 cases and which are assumed to be the closest to the Orano TN industrial cases are reported in Figure 6 with their C_k values. The latter were determined using the TSUNAMI-IP sequence of the SCALE package. The C_k parameter[a] uses information from the sensitivity coefficients of both the Orano TN case and the selection of benchmarks, as well as the covariance matrix to characterize the similarity.

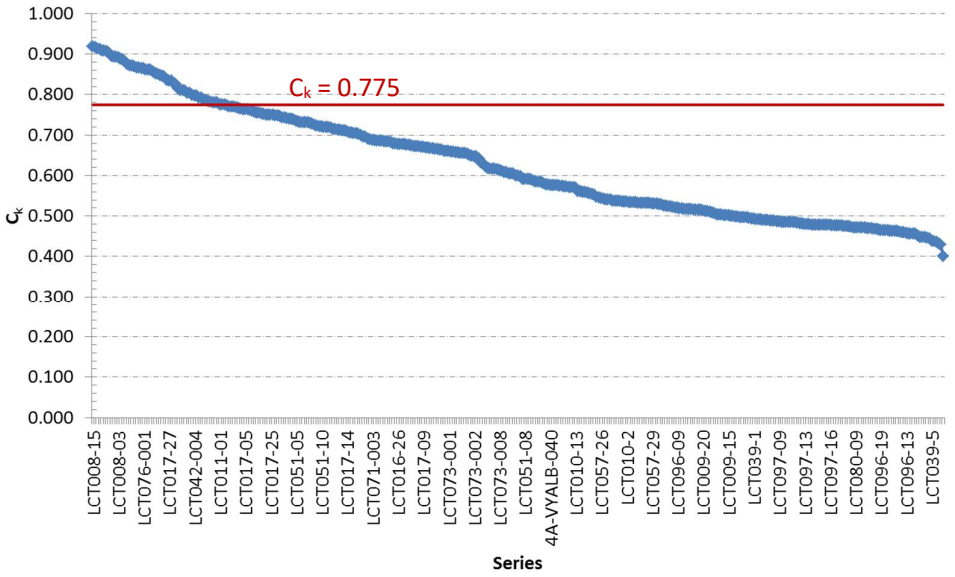

Figure 6 C_k value on a selection of benchmarks from the 361 initial cases

6.2.3 Bias evaluation

A restricted selection of 40 benchmark experiments was used for evaluating the bias due to nuclear data on the Orano TN industrial case. It corresponds to a limit of 0.775 on the C_k value and allows the incorporating of the experiments that were judged to be close to the Orano TN industrial case from an expert judgment. For that selection, a good match between the selected experiments and the benchmarks was obtained. The corresponding average C-E is -55 pcm and the associated standard deviation from the mean is 230 pcm.

No correlation between experiments was retained, which is a strong assumption. The reason is that the correlations are not known and would have needed to be calculated.

This assimilation of data strongly reduced the amount of uncertainty pertaining to the nuclear data from 440 pcm to 120 pcm for both Orano cases considering the ENDF/B-VII.1 covariance matrix.

The bias due to nuclear data after the data assimilation process was assessed as being negligible: 41 pcm ± 118 pcm for case 1, and 5 pcm ± 107 pcm for case 2.

6.2.4 Comparison of methods

Table 4 gives the values of the bias and its associated uncertainties obtained for cases1 and 2 using expert judgment and the GLLSM methodology. The expert judgment method and the GLLSM methodology are both consistent in terms of determination of the bias and its associated uncertainties for the two industrial Orano TN configurations. Both methods result in a negligible bias (lower than 100 pcm). Moreover, as no bias can be attributed to the calculation options, since a continuous energy Monte Carlo code is used, all the biases are therefore due to the nuclear data.

Table 4 Summary of results

	Case 1		Case 2	
Methodology	**Bias**	**Uncertainty**	**Bias**	**Uncertainty**
Expert judgment (pcm)	-13	+208	-13	+208
GLLSM (pcm)	+41	+118	+5	+107

CONCLUSIONS

The study described in this paper compared two different approaches to assess the code bias and its associated uncertainty through a given Orano TN transport and storage cask. The results obtained with both the expert judgment method and the GLLSM methodology combined with sophisticated calculation tools are consistent. Critical experiments close to the industrial configurations were determined and both methods led to a negligible bias (lower than 100 pcm). In addition, since a continuous energy Monte Carlo code was used in the criticality calculation, the bias is mainly due to nuclear data. It is also important to notice that the conclusion of this study is only applicable to the ENDF/B-VII.1 nuclear data library. Indeed, the GLLSM methodology depends mainly of the covariance matrix. Therefore, the same exercise should be performed for all other nuclear data libraries.
Finally, with the feedback from this study, it would be interesting to test the same approach on other industrial configurations or to use other sensitivity/uncertainty calculation tools (e.g. the IRSN MACSENS tool).

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[a] $C_k = \frac{{}^tS_k \times C \times S_E}{\sqrt{{}^tS_k \times C \times S_k} \times \sqrt{{}^tS_E \times C \times S_E}}$ with where S_k is the sensitivity to the application case and S_E the sensitivity of the selected experiment, ${}^tS_k$ and ${}^tS_E$ being the transpose matrices of S_k and S_E, C being the covariance matrix.

Please note that this coefficient is strongly dependent on the covariance data; it provides feedback on nuclear data more than it gives an idea of the similarity.