UACSA PHASE IV: ROLE OF INTEGRAL EXPERIMENT COVARIANCE DATA FOR CRITICALITY SAFETY VALIDATION
SUMMARY OF SELECTED RESULTS

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ABSTRACT

The subject of UACSA Phase IV was the quantification of covariances between neutron multiplication factors k_{eff} *of criticality safety benchmark experiments due to uncertainties of system parameters shared by different experiments and the investigation of the impact of these covariances on criticality safety validation. Generally, these covariances have an impact on the computation of the* k_{eff} *bias and its uncertainty and, hence, on the best estimate plus uncertainty* k_{eff} *prediction for a given application case. Phase IV was divided into two sub-phases named as Phase IVa and Phase IVb. Phase IVa was based on an analytic toy model while Phase IVb was based on a set of critical experiments from the ICSBEP handbook. In both sub-phases, the task was to calculate the covariances and apply them to estimate the bias-corrected* k_{eff} *values of given application cases. In this paper we focus on the results for the bias-corrected* k_{eff} *values. A comprehensive summary of all exercise results will be presented in the final report on Phase IV.*

KEY WORDS

Uncertainty Analysis, Integral Experiment Covariances, Criticality Safety Validation.

1. INTRODUCTION

The summary and results presented in this work are based on an exercise (Phase IV) proposed by the Expert Group on Uncertainty Analysis for Criticality Safety Assessment (UACSA) under the guidance of the Working Party on Nuclear Criticality Safety (WPNCS) of the OECD-NEA [1]. A report with full details and discussion of the results will become available [2].

Covariances between neutron multiplication factors k_{eff} of benchmark experiments are caused by uncertainties of shared system parameters for experiments belonging to the same experimental series[1]. For example, in a series of fuel lattice experiments the same fuel rods are generally used in different experimental arrangements, and all experiments belonging to this series are impacted by the same manufacturing tolerances of the fuel rods. This leads to non-vanishing covariances between the benchmark k_{eff} values estimated from the experiment specifications. UACSA Phase IV consisted of two sub-phases: A simple analytic toy model exercise (Phase IVa), and a more realistic exercise (Phase IVb), involving fuel lattice experiments from the LEU-COMP-THERM-007/039 experimental series documented in the ICSBEP handbook [3]. For both sub-phases, the objective was to estimate for a series of benchmark experiments the covariance matrix of neutron multiplication factors due to system parameter uncertainties and to quantify the impact of these covariances on the k_{eff} prediction (best estimate and uncertainty) of an application case.

The motivation for including the toy model exercise (Phase IVa) was that it constitutes a simple and well-defined problem to apply the same computational steps that must be performed for a realistic application case. This gives the opportunity for a clean comparison between different computational approaches.

For the realistic exercise (Phase IVb), the calculations should be performed using computational tools typically used for licensing cases. The Phase IVb proposal included three different application cases: a water-moderated PWR fuel assembly, and two experiments from the LEU-COMP-THERM-079 (LCT-79) benchmark experiment series.

In the following, we will review the results for the bias-corrected k_{eff} values of the Toy Model and Application Case 1 from LCT-79. For further results, especially for the evaluation of the different correlation matrices, we refer to [2].

2. PHASE IVa: ANALYTIC TOY MODEL

The first exercise (Phase IVa) of UACSA Phase IV was related to a simple analytic toy model. The tasks of this exercise were envisaged to not require the development of sophisticated mathematical tools but to be solved by a simple approach, e.g., by using a spreadsheet application. A broader discussion and definition of the Toy Model can be found in [1].

For simplicity, the Toy Model assumed that any nuclear fuel system is completely defined by a three-dimensional system parameter vector[2] $\boldsymbol{x} = (x_1, x_2, x_3)^T$. For given system parameters $\boldsymbol{x}$, the calculated k_{eff} value k_C is given by

$$k_C(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}) = \frac{\hat{\alpha}_1 \hat{\alpha}_4 x_1}{\hat{\alpha}_1 x_1 + \hat{\alpha}_2 x_2 + \hat{\alpha}_3 x_3}, \tag{1}$$

with

$$\hat{\boldsymbol{\alpha}} = (\hat{\alpha}_1, \hat{\alpha}_2, \hat{\alpha}_3, \hat{\alpha}_4)^T = (9.9968, 1.0066, 1.0225, 1.2198)^T \,. \tag{2}$$

The parameter vector $\hat{\boldsymbol{\alpha}}$ is assumed to be derived from some nuclear data evaluation. $\hat{\boldsymbol{\alpha}}$ is supposed to be the best estimate of the unknown vector $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3, \alpha_4)^T$ corresponding to the true nuclear data. The uncertainties and correlations related to the estimation of $\boldsymbol{\alpha}$ are expressed by the covariance matrix:

$$\boldsymbol{\Sigma}_{\boldsymbol{\alpha}} = \begin{pmatrix} \sigma_{\alpha_1}^2 & 0 & 0 & 0 \\ 0 & \sigma_{\alpha_2}^2 & 0 & 0 \\ 0 & 0 & \sigma_{\alpha_3}^2 & 0 \\ 0 & 0 & 0 & \sigma_{\alpha_4}^2 \end{pmatrix} = 10^{-4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3}$$

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[1] Covariances may be affected by simplifications of the experiment specifications. However, an analysis of such effects is beyond the scope of this exercise.

[2] Please note that the considered toy model is not supposed to have any physical meaning.

Since $\boldsymbol{\Sigma}_{\boldsymbol{\alpha}}$ is diagonal, the estimates of α_1 through α_4 are uncorrelated. The parameters $\sigma_{\alpha_1}^2$ through $\sigma_{\alpha_4}^2$ may be interpreted as variances of normal distribution models reflecting the uncertainties in the estimation of α_1 through α_4, respectively.

Table I contains the best estimate values of the system parameters x_1, x_2 and x_3 of nine different benchmark experiments and their corresponding standard deviations σ_1, σ_2 and σ_3. These best estimates and standard deviations may be interpreted as mean values and standard deviations of normal distribution models, respectively.

Table I: System parameters and corresponding 1-σ errors of nine different benchmark experiments

ID	x_1	σ_1	x_2	σ_2	x_3	σ_3	$k_C(x,\hat{\alpha})$	k
Experiment 1	**2.0072**	**0.05**	**4.0424**	**0.05**	**-0.0746**	**0.05**	**1.0174**	**1.0**
Experiment 2	**2.0072**	**0.05**	**1.9601**	**0.05**	**1.9292**	**0.05**	**1.0194**	**1.0**
Experiment 3	**2.0072**	**0.05**	**-0.0506**	**0.05**	**3.9477**	**0.05**	**1.0177**	**1.0**
Experiment 4	**2.0072**	**0.05**	**-2.0458**	**0.05**	**6.0650**	**0.05**	**1.0111**	**1.0**
Experiment 5	**2.0072**	**0.05**	**-3.9905**	**0.05**	**8.0370**	**0.05**	**1.0086**	**1.0**
Experiment 6	**2.0072**	**0.05**	**-6.0613**	**0.05**	**9.8448**	**0.05**	**1.0185**	**1.0**
Experiment 7	**2.0072**	**0.05**	**-12.0059**	**0.05**	**15.9819**	**0.05**	**1.0063**	**1.0**
Experiment 8	**2.0072**	**0.05**	**-16.0923**	**0.05**	**19.9995**	**0.05**	**1.0066**	**1.0**
Experiment 9	**2.0072**	**0.05**	**-20.0440**	**0.05**	**23.9692**	**0.05**	**1.0032**	**1.0**

The second-to-last column contains the calculated k_{eff} values according to Eq. (1), and the last column contains the experimental k_{eff} values k. Here, the errors related to the k_{eff} measurements are assumed to be negligible. Hence, the k values may be regarded as the true neutron multiplication factors of the respective benchmark experiments.

The best estimate values of the system parameters x_1, x_2, and x_3 and of the four nuclear data values $\hat{\boldsymbol{\alpha}}$ were generated from their specified uncertainty distributions, using their true values (known to the author of the Toy Model but unknown to the participants) as a basis. The true values are given by $\boldsymbol{\alpha} = (1.0,1.0,1.0,1.2)^T$. The true values of the system parameters x_1, x_2, and x_3 are obtained by rounding the estimated values in Table I to the nearest integer values.

In the following, we describe and discuss the received solutions for Task 2. For the description and discussion of the results obtained for Task 1 we refer to [2].

Task 2 was about estimating the bias-corrected k_{eff} value and quantifying the uncertainty of this estimation for the application case defined by the system parameter vector $\boldsymbol{x} = (1.5,-6,10)^T$. For Task 2a, it was assumed that there is no stochastic dependence between the system parameter vectors $\boldsymbol{x}$ of different benchmark experiments (e.g., due to independent production processes). For Task 2b, on the other hand, it was assumed that system parameter x_1 is the same for all nine benchmark experiments (i.e. all nine experiments have a common component).

We were able to evaluate 9 results (Evaluations A1 to H) for Tasks 2a and b, respectively.

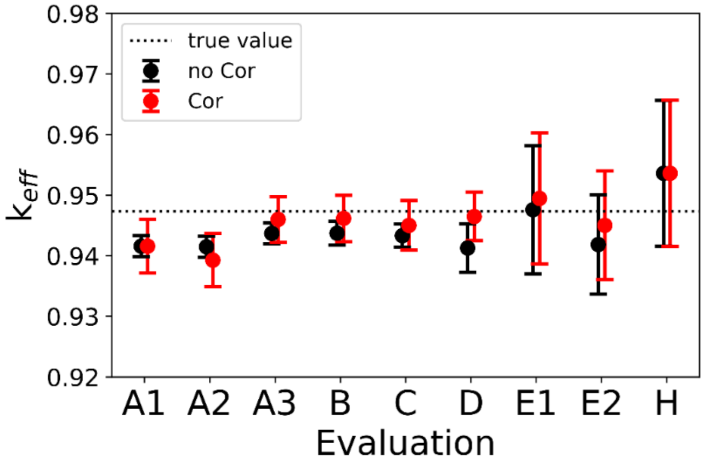

Figure 1: Graphic presentation of results for the Toy-Model. The dotted line represents the (unknown) true value of k_{eff} = 0.9474. The black values represent the uncorrelated case, and the red values the correlated case. The error bars indicate the 1-σ uncertainties.

The objective of the toy model was to analyze the impact of different methods to evaluate covariance / correlation data and to predict the bias-corrected k_{eff} values.

The results for the bias-corrected k_{eff} values for Task 2 show generally a good agreement. Most results for the correlation case reproduce the true k_{eff} value within 1-σ uncertainty. Only the results A1 and A2 and the non-correlation results of B, C, and D show a larger than 1-σ deviation. Further, it can be observed for the correlation case that the mean values of B, C, D, E1, and E2 are larger compared to the non-correlation case. The results of H show no difference between the assumption of correlation and non-correlation: The mean values and 1-σ uncertainties are statistically compatible.

It is notable that the solutions A, B, C, and D have significantly smaller 1-σ uncertainties compared to the results E and H. The larger 1-σ uncertainties of solutions E and H might be because frameworks were used in which only the mean value but not the standard deviation is updated. The results A3 and B are essentially the same because they were obtained using the same method.

Generally, it can be observed that taking correlations correctly into account leads to better agreement between predicted and true k_{eff} values.

3. PHASE IVb: REALISTIC CASE: EXPERIMENTS WITH WATER-REFLECTED UO_2 FUEL ROD ARRAYS

Phase IVb was based on 21 criticality safety benchmark experiments, evaluated in [3]. Four experiments were taken from series LEU-COMP-THERM-007 (LCT-007), namely experiments 1 to 4. The remaining 17 experiments were taken from LEU-COMP-THERM-039 (LCT-039). All experiments of LCT-007 and LCT-039 were carried out in the “Apparatus B” facility at the CEA (Commissariat à l’Energie Atomique et aux Energies Alternatives) Valduc Criticality Laboratory in 1978; for details see [4, 5].

To receive a better comparability of results, the data given in the ICSBEP handbook was supplemented by further information, including the distribution models used to express the uncertainties of the considered parameters. This data is summarized in Table II. Additional considerations were made to describe the positions of the fuel rods in the holes of the grid plate; see Figure 2. The modelling scenarios A to E summarized in Table III differ with regard to different assumptions about the correlations between the fuel rod parameters of different fuel rods and the fuel rod positions within the grid holes.

Table II: System parameters and their uncertainties. **U(a,b) denotes a uniform distribution function between a and b; N(μ,σ²) denotes a normal distribution function with expectation value μ and variance σ².**

Parameter	Distribution Model	Model Parameters
Fuel rod cladding inner diameter	$U(a,b)$	a = 0.81 cm, b = 0.83 cm
Fuel rod cladding thickness	$U(a,b)$	a = 0.055 cm, b =0.065 cm
Fuel pellet diameter	$N(\mu,\sigma^2)$	μ = 0.7892 cm, σ = 0.0017 cm
x-displacement of hole position relative to nominal hole position (see Eq. (4.2))	$N(\mu,\sigma^2)$	μ = 0 cm, $\sigma = 0.0105\ cm/\sqrt{2} \cong 0.00742$ cm
y- displacement of hole position relative to nominal hole position (see Eq. (4.3))	$N(\mu,\sigma^2)$	μ = 0 cm, $\sigma = 0.00742$ cm
Angle θ fixing position of rod center within its grid hole	$U(a,b)$	a =0, b =2π.
Hole diameter	$N(\mu,\sigma^2)$	μ = 1.0105 cm, σ = 0.0085 cm
Height of fissile column	$N(\mu,\sigma^2)$	μ = 89.7 cm, σ = 0.3 cm
Fuel density	$N(\mu,\sigma^2)$	μ = 10.38 g/cm^3, σ = 0.0133 g/cm^3
Fuel impurity (atomic density of ^{10}B)	$N(\mu,\sigma^2)$	$\mu = 6.9037\times10^{-8}$ atom/(barn·cm), $\sigma = 8.0000\times10^{-9}$ atom/(barn·cm)
^{234}U content in U	$N(\mu,\sigma^2)$	μ = 0.0307 At.-%, σ = 0.0005 At.-%
^{235}U content in U	$N(\mu,\sigma^2)$	μ = 4.79525 At.-%, σ = 0.002 At.-%
^{236}U content in U	$N(\mu,\sigma^2)$	μ = 0.1373 At.-%, σ = 0.0005 At.-%
^{238}U content in U	$N(\mu,\sigma^2)$	μ = 95.03675 At.-%, σ = 0.01 At.-%
Critical water height LCT-07-01	$N(\mu,\sigma^2)$	μ = 90.69 cm, σ = 0.1 cm
Critical water height LCT-07-02	$N(\mu,\sigma^2)$	μ = 73.53 cm, σ = 0.1 cm
Critical water height LCT-07-03	$N(\mu,\sigma^2)$	μ = 77.98 cm, σ = 0.06 cm
Critical water height LCT-07-04	$N(\mu,\sigma^2)$	μ = 79.85 cm, σ = 0.1 cm
Critical water height LCT-39-01	$N(\mu,\sigma^2)$	μ = 81.36 cm, σ = 0.07 cm
Critical water height LCT-39-02	$N(\mu,\sigma^2)$	μ = 77.69 cm, σ = 0.06 cm
Critical water height LCT-39-03	$N(\mu,\sigma^2)$	μ = 73.05 cm, σ = 0.06 cm
Critical water height LCT-39-04	$N(\mu,\sigma^2)$	μ = 89.07 cm, σ = 0.06 cm
Critical water height LCT-39-05	$N(\mu,\sigma^2)$	μ = 84.37 cm, σ = 0.06 cm
Critical water height LCT-39-06	$N(\mu,\sigma^2)$	μ = 58.77 cm, σ = 0.06 cm
Critical water height LCT-39-07	$N(\mu,\sigma^2)$	μ = 69.71 cm, σ = 0.06 cm
Critical water height LCT-39-08	$N(\mu,\sigma^2)$	μ = 66.79 cm, σ = 0.06 cm
Critical water height LCT-39-09	$N(\mu,\sigma^2)$	μ = 64.47 cm, σ = 0.07 cm
Critical water height LCT-39-10	$N(\mu,\sigma^2)$	μ = 58.37 cm, σ = 0.07 cm
Critical water height LCT-39-11	$N(\mu,\sigma^2)$	μ = 81.34 cm, σ = 0.06 cm
Critical water height LCT-39-12	$N(\mu,\sigma^2)$	μ = 75.38 cm, σ = 0.07 cm
Critical water height LCT-39-13	$N(\mu,\sigma^2)$	μ = 72.52 cm, σ = 0.06 cm
Critical water height LCT-39-14	$N(\mu,\sigma^2)$	μ = 71.14 cm, σ = 0.06 cm
Critical water height LCT-39-15	$N(\mu,\sigma^2)$	μ = 69.88 cm, σ = 0.06 cm
Critical water height LCT-39-16	$N(\mu,\sigma^2)$	μ = 69.4 cm, σ = 0.06 cm
Critical water height LCT-39-17	$N(\mu,\sigma^2)$	μ = 68.75 cm, σ = 0.06 cm

Table III: Scenarios defined by different assumptions about the correlations between the fuel rod parameters of different fuel rods and the fuel rod positions within the grid holes.

Scenario	Displacement of grid hole position	Radial displacement of rod center from the hole center	Grid hole diameters	Fuel rod cladding inner diameters	Fuel rod cladding thicknesses
A	None	$R = 0$	Correlated	Correlated	Correlated
B	Uncorrelated	$R = r_{\text{hole}} - r_{\text{gap}} - t_{\text{clad}}$	Correlated	Correlated	Correlated
C	Uncorrelated	$R = r_{\text{hole}} - r_{\text{gap}} - t_{\text{clad}}$	Uncorrelated	Correlated	Correlated
D	Uncorrelated	$R = r_{\text{hole}} - r_{\text{gap}} - t_{\text{clad}}$	Uncorrelated	Uncorrelated	Correlated
E	Uncorrelated	$R = r_{\text{hole}} - r_{\text{gap}} - t_{\text{clad}}$	Uncorrelated	Uncorrelated	Uncorrelated

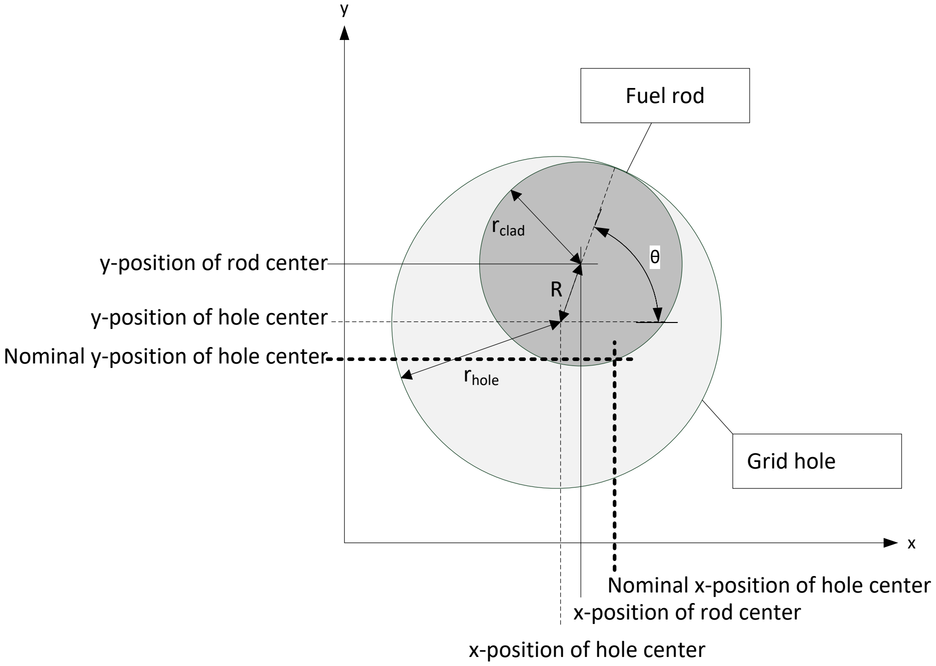

Figure 2: Positioning of fuel rod within its grid hole

The results presented here are based on the assumptions related to Scenario A (strong correlation), Scenario E (lower correlation) and the assumption of no correlations. The participants evaluated the corresponding uncertainties, covariance and correlation coefficients for each of the three modelling assumptions (strong, lower, and no correlation) for the 21 experiments from the ICSBEP handbook. For the details of these evaluations, we refer to [2].

In a next step, the importance of accounting for the integral experiment correlations in a criticality safety validation was investigated. The aim was to quantify the impact of the correlations on the prediction of the bias-corrected k_{eff} value and its related uncertainty for the given application cases.

Here we present the results for Application Case 1, specified in detail in [1]. For this application case, a simplified 16×16 PWR fuel assembly was considered. The specification included the positions of the 236 fuel rods and 20 guide thimbles, as well as the system parameter values and their corresponding uncertainties. Any additional materials, such as the assembly foot, assembly head and spacer grids were neglected. Only the uncertainties in the fuel rod and guide thimble dimensions and in the height of the fuel column were considered.

The task was to calculate the bias-corrected k_{eff} values and their related uncertainties based on the results of the covariances generated for the 21 benchmark experiment configurations.

A total of nine different sets of results for the bias-corrected k_{eff} values of Application Case 1 were received. Six results were received for the bias-corrected k_{eff} value neglecting correlations, eight results accounting for strong correlations following Scenario A, and six results accounting for lower correlations (Scenario E). The expression *strong correlations* refers here to Pearson's correlation coefficients around 0.98. The actual values for the *lower correlations* vary between 0.1 and 0.8 depending on the assumptions made by the participants during the evaluation process. For the details of the correlation matrices and the related discussion we refer to [2].

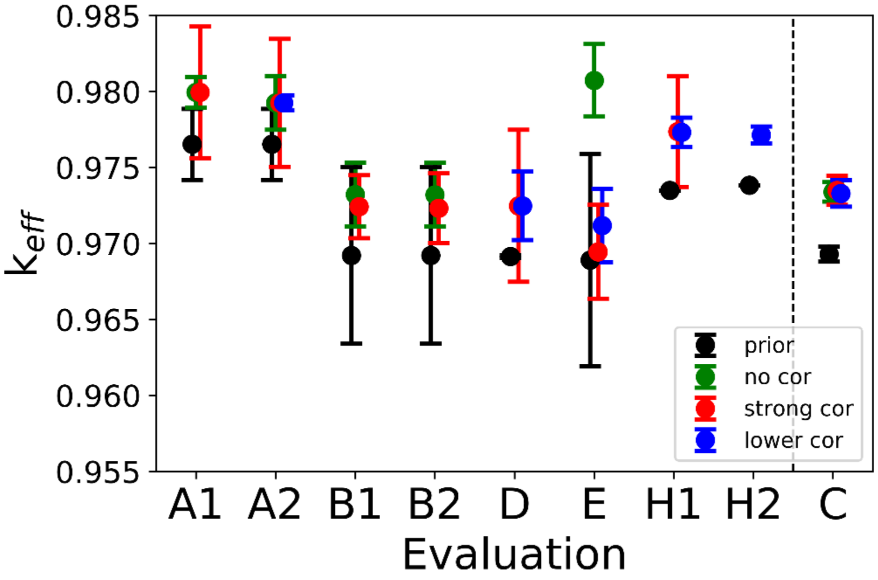

Figure 3: Results for Application Case 1. Note that the results for Participant C are based on an earlier Phase IVb definition.

The calculated prior k_{eff} values for Application Case 1 can be divided into two groups. Participants A and H calculated higher values than Participants B, D, E, and C. All results show an increase for the bias-corrected k_{eff} values and a decrease of the 1-σ interval, except for the bias-corrected values of Participant A assuming strong correlation. It is notable that the results for the bias-corrected k_{eff} values are comparable for both definitions of Phase IVb.

The bias-corrected values of Participants B, D, E, and C all agree within one sigma. The same is true for the bias-corrected values of A, H, and the no-correlation value of Participant E. Except for the latter, the discrepancies can be explained by the different "starting points" of the analysis, i.e. the prior k_{eff} values, which can probably be attributed to differences in the criticality calculation models. Since the bias-corrected values rely on the prior estimations, different prior estimations lead to different bias-corrected values.

4. CONCLUDING REMARKS AND OUTLOOK

We presented a selection of results from the UACSA Phase IV exercise. The objective of Phase IV was to test methodologies to express the joint variability between benchmark neutron multiplication factors in terms of covariances and to evaluate the impact of these covariances on the predictions of the bias-corrected neutron multiplication factors. Two different exercises were considered: an analytic toy model exercise

(Phase IVa), and a realistic exercise (Phase IVb) involving experiments with water-reflected UO_2 fuel rod arrays. Please note that the results are discussed in great detail in [2]. This includes also detailed discussions of the covariance and correlation matrices the participants derived. For the article at hand we limit ourselves to discussions of the variation of the resulting k_{eff} values.

For the Toy Model, we evaluated nine different results by six participants. Taking into account the correlation effects, most results for the bias-corrected k_{eff} value were in good agreement with one another, and the true k_{eff} value was mostly reproduced within one standard deviation.

For Application Case 1 of the realistic exercise, the results by six participants were analyzed. Six results included the k_{eff} values for the ”no-correlation” and “strong correlation” scenario. Except for discrepancies attributable to differences in the criticality calculation models, the results were in reasonably good agreement with one another. Only one result showed a clear difference from the other results (see Figure 3).

In this context, it must be noted that in Phase IVb the bias-corrected k_{eff} values and their uncertainties were the results of lengthy calculation chains involving individual assumptions. Differences between assumptions sometimes led to considerable differences between the estimated covariances, sensitivities and k_{eff} uncertainties which again led to noticeable differences between the results of the bias-corrected k_{eff} values. This was the case even though the information on the criticality benchmark experiments in the ICSBEP handbook was supplemented by additional information in the Phase IVb specification in order to avoid ambiguities. For a more detailed discussion we refer to [2].

A general conclusion that can be drawn from UACSA Phase IV is that integral experiment covariances can have an important impact on the calculation of bias-corrected neutron multiplication factors and their uncertainties. They should, therefore, generally be considered in criticality safety validation.

We recommend further investigations based on far simpler and unambiguous exercise definitions in which no user specific biases conflict any comparison. Based on the results obtained for UACSA Phase IV it appears to be impossible to draw general statements on the methodologies to express the joint variability between benchmark neutron multiplication factors in terms of covariances and on the evaluation of the impact of these covariances on the predictions of the bias-corrected neutron multiplication factors.

It should be underlined that UACSA Phase IV and the related discussions in- and outside of the WPNCS led to an awareness of the problems and the development of different methodologies to account for shared uncertainties and covariances between benchmark experiments.

ACKNOWLEDGMENTS

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