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Modeling of critical experiments and its impact on integral covariance matrices and correlation coefficients

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ABSTRACT

In this manuscript we study the modeling of experimental data and its impact on the resulting integral experimental covariance and correlation matrices. By investigating a set of three low enriched and water moderated UO_2 fuel rod arrays we found that modeling the same set of data with different, yet reasonable assumptions concerning the fuel rod composition and its geometric properties leads to significantly different covariance matrices or correlation coefficients. Following a Monte Carlo Sampling approach, we show for nine different modeling assumptions the corresponding correlation coefficients and sensitivity profiles for each pair of the effective neutron multiplication factor k_{eff}. Within the 95% confidence interval the correlation coefficients vary from 0 to 1, depending on the modeling assumptions. Our findings show that the choice of modeling can have a huge impact on integral experimental covariance matrices. When the latter are used in a validation procedure to derive a bias, this procedure can be affected by the choice of modeling assumptions, too. The correct consideration of correlated data seems to be inevitable if the experimental data in a validation procedure is limited or one cannot rely on a sufficient number of uncorrelated data sets, e.g. from different laboratories using different setups.

1. Introduction

Criticality safety assessments require a prediction of the effective neutron multiplication factor (k_{eff}) below a sufficient safety margin. This predicted value is derived using a validated calculation method with validated computer codes, e.g. so called criticality codes to calculate the k_{eff} of an application case. The validation of a criticality code can be achieved by recalculations of suitable critical experiments performed in laboratories and documented and evaluated e.g. in NEA Nuclear Science Committee (2010). In recent years, several authors discussed the fact that depending on the application case and the choice of experiments, the effect of correlated experimental data on the determination of the bias, its uncertainty, and the resulting safety margins has to be considered (Ivanova et al., 2003; Bock et al., 2013a,b; Hoefer et al., 2015a; Peters et al., 2015a,b; Sobes et al., 2015; Marshall et al., 2015; Baker et al., 2015). The questions arising in the field of determination and handling of integral experimental covariance matrices in the process of code validation are also discussed in the Expert Group on Uncertainty Analysis for Criticality Safety Assessment (UACSA), a sub-group of the Working Party on Nuclear Criticality Safety (WPNCS) of the Nuclear Energy Agency (NEA) within the Organization for Economic Co-operation and Development (OECD). Actual questions which arose recently are: How to treat given sets of similar experimental data without knowing all exact statistical dependencies; and further, what are the implications on modeling these experiments in a code validation procedure regarding the consideration of the complete integral experimental correlation or covariance matrices?

In this manuscript we address these questions by following parts of the groups proposal for a benchmark called Role of Integral Experiment Covariance Data for Criticality Safety Validation (Hoefer et al., 2015b). In contrast to the benchmark proposal we focus on a reduced number of experiments but a total of nine different modeling approaches.

With the following analysis we add a new perspective to the discussion and show the effect of different modeling approaches for the same set of experimental data on the resulting integral covariance or correlation matrices.

Correlated data can arise if different experiments share parts of the experimental setup, measurement systems, or other relevant parameters. Some experiments described in the ICSBEP are not performed as single experiments, but slight variations of a setup were repeatedly investigated and published as a series of the same experiment. This is e.g. the case for LEU-COMP-THERM-039

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(LCT-39), where the number and location of empty positions in a fuel rod grid were varied. In the following work we focus on the experimental data from experiments numbers 6, 7, and 8 from this series described in detail in NEA Nuclear Science Committee (2010), Hoefer et al. (2015b) and Peters et al. (2015a) and references therein. The critical experiments consist of water moderated low enriched uranium fuel rods with a thermal neutron spectrum. The experimental setups are 22×22 arrays consisting of 363 (459, 448) fuel rods for experiment 6 (7, 8) and 121 (25, 36) empty spots, respectively. For further details we refer to NEA Nuclear Science Committee (2010) and Peters et al. (2015a). Clearly these experiments share certain components, and treating them as individual statistical independent data sets in the process of validation probably would not be appropriate. Hence, the determination of the integral covariance or correlation matrix of the experiments is a crucial step on the way to determine a bias of the calculated application case k_{eff}.

2. Methods and parameters

For the determination of the integral covariance matrices of k_{eff} and the corresponding correlation matrices we use a Monte Carlo Sampling approach, and SUnCISTT (Behler et al., 2014) to steer and evaluate the numerous SCALE 6.1.2 (SCALE, 2012) calculations. For two sets A and B of n sampled neutron multiplication factors k_{eff}, the covariance cov^{AB} is defined as

$$\text{cov}^{AB} = \frac{1}{n-1}\sum_{i=1}^{n}\left(k_{\text{eff}}{}^{A,i} - \overline{k_{\text{eff}}}^{A,i}\right)\left(k_{\text{eff}}{}^{B,i} - \overline{k_{\text{eff}}}^{B,i}\right) \tag{1}$$

with $\overline{k_{\text{eff}}}$ symbolizing the expectation value of k_{eff}, in our case the sample mean. The covariance can be interpreted as a measure of how much the k_{eff} of the two sets change simultaneously. A positive covariance indicates the following monotonic connection between the two sets: large (or low) values in A correspond to large (or low) values in B. A negative covariance indicates the opposite behavior: large values in A correspond to low values in B. Due to its linearity the covariance gives only a tendency of the connection of two sets of random variables. To get comparable statements for more than two sets the covariance can be normalized with the standard deviation σ to get the correlation coefficient cor:

$$\text{cor}^{AB} = \frac{1}{\sigma_A \sigma_B}\text{cov}^{AB} \tag{2}$$

The correlation coefficient is a dimensionless measure of the linear dependence of two sets of random variables and takes values between +1 (complete positive linear connection) and −1 (complete negative linear connection). The confidence interval around the calculated cor is due to the value limitation of cor non-symmetric and must be determined by using transformations to so called Fishers distribution z (Fisher, 1915). The latter is almost normally distributed and depends on the sample correlation coefficient:

$$z(\text{cor}) = \frac{1}{2}\ln\left(\frac{1+\text{cor}}{1-\text{cor}}\right) \tag{3}$$

The corresponding tolerance intervals are calculated via $z \pm \text{CL} \times \delta$ with the confidence level CL (e.g. 1.96 for the 95% confidence interval) and the sample standard deviation $\delta = \sqrt{(n-3)^{-1}}$. The resulting z values are then transformed back to cor values. All given confidence intervals in the following work are 95% intervals.

Following a Monte Carlo Sampling approach, each value describing the experiment has to be interpreted as a distribution function. This means in turn, that the definition and interpretation of the experimental parameters and their uncertainties is essential. It strongly depends on the quality of the experimental data and availability of precise uncertainty specifications. To circumvent the problem of determining suitable distribution function for each parameter, we apply the ones given in Hoefer et al. (2015b) which are also listed in 1. All experimental parameters are supposed to follow a uniform U(a,b) or normal distribution $\text{N}(\mu, \sigma)$. Assuming the three experiments LCT-39 6, 7, and 8 to be statistical independent gives a correlation coefficient close to zero. Results for this assumption are shown for the correlation of k_{eff} values calculated by KENO V.a using the parameters given in Table 2 for 250 Monte Carlo samples for each experiment. The underlying model assumptions for the results of Fig. 1 are very simple and straight forward: It is assumed, that the fuel rods are all identical in composition and position within its unit cell. In consequence, the modeling of one experiment consists basically of a 22×22 array of identical unit cells for the fuel rods and the empty positions respectively. (see Tables 1 and 3).

Table 1
All model parameters and their distribution characteristics, following the suggestions of the benchmark proposal (Hoefer et al., 2015b).

Model parameters	Type of variation	Distribution functions
Fuel diameter [cm]	Depends on scenario	N(0.7892, 0.0017)
Fuel lengths [cm]	Depends on scenario	N(89.7, 0.3)
Fuel density [g/cm^3]	Depends on scenario	N(10.38, 0.0133)
Fuel content 234U[At.-%]	Depends on scenario	N(0.0307, 0.0005)
Fuel content 235U [At.-%]	Depends on scenario	N(4.79525, 0.002)
Fuel content 236U[At.-%]	Depends on scenario	N(0.1373, 0.0005)
Boron concentration [atom/barn × cm × 10^{-8}]	Depends on scenario	N(6.9037, 0.8)
Critical water height [cm]	Individual	N(μ, σ) dep. on experiment
Angle of fuel rod	Individual	U(0, 2π)
Offset of grid hole x [cm]	Individual	N(0, 0.00742)
Offset of grid hole y [cm]	Individual	N(0, 0.00742)
Hole diameter [cm]	Depends on scenario	N(0.0105, 0.0085)
Inner cladding diameter [cm]	Depends on scenario	U (0.81, 0.83)
Cladding thickness [cm]	Depends on scenario	U (0.055, 0.065)

Table 2
Used codes and cornerstones of calculations. KENO V.a is taken from the CSAS5 sequence of SCALE 6.1.2.

Code	Parameter	Value
KENO V.a	Nuclear data library	ENDF/B-VII (ce)
	Neutrons per generation	10,000
	Skipped generations	500
	σ_{MC}	5×10^{-4}(Sc. A to D); 1×10^{-4}(Sc. E to H)
SUnCISTT	Number of samples	250

3. Modeling assumptions

Having determined all relevant parameters and their distribution functions, a calculation model is built to calculate the neutron transport equations and determine the neutron multiplication factor. Obviously the model should be as close as possible to the