# CALCULATING UNCERTAINTY ON K-EFFECTIVE WITH MONK10

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## ABSTRACT

Criticality safety assessments require a demonstration that a particular configuration of fissile material has an adequate sub-critical margin (*k-effective* sufficiently below unity) to ensure that the risk of criticality under normal operation and accident conditions is acceptable. The required sub-critical margin depends upon the uncertainty in the estimated value of *k-effective*. The uncertainty in the calculated value of *k-effective* arises from a number of sources, including: manufacturing tolerances on input data to the code (affecting geometry, compositions and densities), uncertainty in the nuclear data used by the code, stochastic uncertainty resulting from Monte Carlo simulation and modelling approximations/errors, including the inevitable bugs in the software.

The ANSWERS Software Service, in collaboration with industrial partners, is developing a number of techniques to better understand and quantify uncertainty on predicted values of *k-effective*, using MONK. The SPRUCE utility code has been developed to allow uncertainty to be estimated using sampling methods. This can include the sampling of input parameters (including dimensions, compositions and densities) from statistical distributions. It can also include sampling different nuclear data libraries. A set of nuclear data libraries has been generated for this purpose by sampling from statistical distributions that represent the uncertainties in the published nuclear data evaluated files; a set of libraries has been produced for Latin Hypercube Sampling. By varying the input data and nuclear data, separate and combined uncertainties due to manufacturing tolerances and nuclear data can be derived. By performing least squares fitting on the results it is also possible to estimate the contribution of each of the uncertain inputs and a sensitivity method in MONK can break down the nuclear data uncertainty.

**Monte Carlo, Criticality, Uncertainty Quantification, Sensitivity Analysis**

## 1. INTRODUCTION

This paper describes an uncertainty analysis using MONK10 (MONK10A_RU0) and SPRUCE for a 16x16 fuel lattice with descriptions of sources of uncertainty arising from manufacturing tolerances. MONK10 [1,2] was released in 2014 by the ANSWERS Software Service which is a part of Amec Foster Wheeler. MONK10 is used extensively for criticality safety calculations both within the UK and abroad.

The ANSWERS Software Service also has produced a tool, SPRUCE, which is used to sample nuclear data and input files for uncertainty analysis. The SPRUCE tool has been used in a variety of applications covering both criticality safety and reactor physics.

The methods to determine the uncertainty arising from nuclear data and manufacturing tolerances in this paper are applied to an application test case which is based upon a PWR fuel array placed within water storage. The application uses a mixture of uniformly and normally distributed parameters. The geometry of the application case is shown in Figure 1, with the MONK geometry shown using Visual Workshop (which is the ANSWERS Software Service's pre- and post-processing integrated development environment for MONK and other ANSWERS codes).

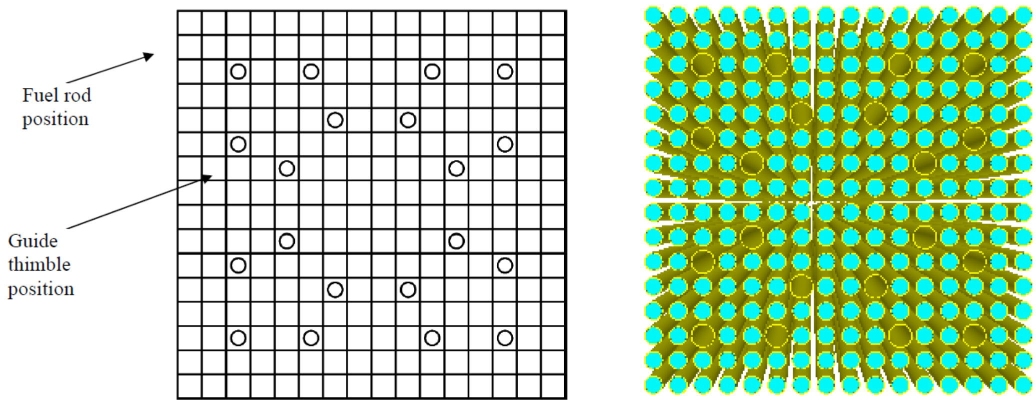


**Figure 1: Left: Geometry for the application case on a 16 x 16 fuel rod lattice. Right: Visual Workshop visualization as used for the MONK10 calculations.**

## 2. METHODS USED IN THE UNCERTAINTY QUANTIFICATION

SPRUCE [3] can be used to sample both nuclear data and input files for a variety of probability distribution functions (PDFs), such as: normal, log-normal, uniform and the beta distribution. The strategy for sampling can be Monte Carlo, stratified sampling or Latin Hypercube Sampling (LHS). In this paper, we use LHS which ensures that the sample space is adequately covered. The use of LHS reduces the number of realisations (individual MONK runs) that are needed to obtain the same variance.

The uncertainty quantification is also used on the nuclear data. MONK uses various collision processors for multigroup (172 WIMS libraries), hyperfine multigroup (DICE) or point energy (BINGO). All calculations in this paper use the JEFF3.1.2 BINGO library.

The methods in SPRUCE are used to sample (using LHS) the JEFF3.1.2 nuclear data together with correlations from JEFF3.1.2 and other sources to form 25 different libraries to cover the sample space. The same methods were used to sample both nuclear data and the manufacturing tolerances within components.

### 2.1. MONK10A Sensitivity Module

MONK10A (also called MONK10 and MONK10A_RU0) is a Monte Carlo code used for criticality safety and reactor physics. The code uses superhistory powering to reduce the correlations from successive stages and concentrate the estimated source at the most reactive regions. Of interest in this paper, is the sensitivity option which MONK includes. MONK uses Differential Operator Sampling (DOS) to estimate the sensitivity and associated stochastic uncertainty to nuclear data. Therefore, it does not need to use the costly addition of many extra runs. The DOS method is strictly speaking a perturbation option, but this can be used for sensitivity analysis. The method focuses on calculating the deviation of the eigenvalue to small changes in the basic nuclear data cross-sections. This size of the deviation is calculated by evaluating,

$$\frac{\sigma}{k}\frac{\partial k}{\partial \sigma} \tag{1}$$

where $k$ is the eigenvalue ($k$-effective) and $\sigma$ is the cross section. The method also calculates the sensitivity to the mean number of neutrons per fission, $\bar{\nu}$. The results can be obtained in specific energy ranges for reaction types, nuclides and materials containing the nuclide.

### 2.2. Sampling using SPRUCE and Latin Hypercube Sampling

SPRUCE can use various sampling methods (such as Monte Carlo, Latin Hypercube and Stratified). For the purposes of this work, we use LHS to ensure that we adequately cover the sample space. The stochastic parameters, in this benchmark, use either a normal or uniform distribution. Each of the subsequent MONK runs was converged to 150pcm (one standard deviation). The basic structure of the process is shown in Figure 2. The run script in the SPRUCE package runs the MONK criticality code.

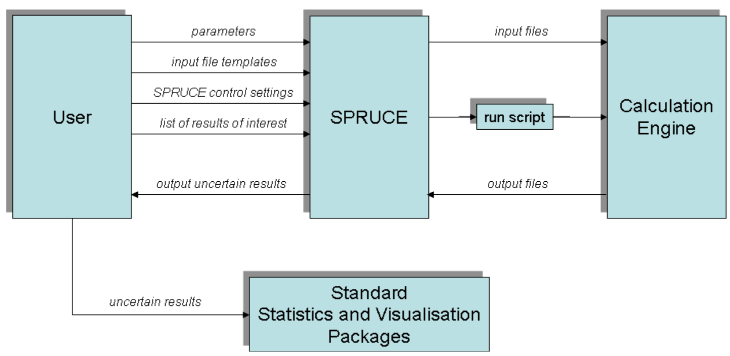


**Figure 2: Schematic of SPRUCE processes**

### 2.3. Calculation of Tolerances

The 97.5% confidence interval describes the reliability of the estimation procedure and gives the confidence that the true value of the multiplication factor is within the upper limit. The one-tailed upper 95%/95% tolerance limit calculates the limit such that 95% of the population falls below this with 95% certainty. The estimate of the confidence and tolerance limit here assumes that the data is normally distributed which can be checked using statistical analysis. The statistical analysis is applied to both the uncertainty in nuclear data and to the uncertainty in the manufacturing tolerances of the various components. The 95%/95% tolerance limit was calculated on the assumption of normally distributed data.

### 2.4. Sensitivity Analysis and Estimation of Bias

The bias from a set of $n$ sampled eigenvalues is estimated by taking the mean value of all of the biases calculated from the individual MONK runs. The standard error method which is used to calculate EPD (Errors in Physical Data) in MONK is also used for this analysis. We also need to calculate two related parameters, namely the correlation and the covariance matrices. The correlation measures the magnitude (strength) of linear relationship between the two random variables.

To estimate the sensitivities of the various components, we use linear regression. Linear regression uses a Least Squares fit to form a linear fit between the independent and dependent variables. We can then take the gradient of the linear equation to approximate the sensitivity.

### 2.5. MONK Categorisation System

MONK has an extensive validation database including a large number of Uranium compound systems. MONK also has an automatic classification system designed to aid in choosing suitable validation cases from the database. It aims to identify a manageable set of properties which can adequately differentiate the neutronic behaviour of different system types. Each system is categorised based on six properties:

- Type of fissile nuclide
- Non-fuel absorption
- Leakage (linked to reflection)
- Resonance absorption
- Fast fission
- Hydrogen fuel content

Each property is scored and then partitioned to define a region of the six dimensional property space (which we call a category). Experiments that lie within the same (or a nearby) category have similar neutronic behaviours. The idea is to compartmentalise a criticality safety case so that it can be compared against similar cases. This can be used to calculate the value for EPD calculated from a system which shares the same category number. The categorisation scheme tries to look at various parameters that effect criticality but does not include aspects such as geometry and moderation; it looks at a physics-based objective view. The critically analyst need to apply intelligent reasoning to identify a particular validation case. Cases with an appropriate geometry or moderation can then be selected from the broad category number provided by MONK.

### 2.6. Nuclear Data Uncertainties

The set of 25 perturbed nuclear data libraries were generated using covariance data from various nuclear data evaluations. In order of preference, these are: JEFF3.1, ENDF/B-VII.0, JENDL3.3, JEF2.2, ENDF-B/VI.8 and TENDL2008.

## 3. ANALYSIS OF RESULTS

The analysis of results concentrates upon the application test case (shown in Figure 1) using the uncertainty quantification tools previously discussed. The application test case has a nominal value of *k*-effective calculated by MONK of 0.9689 ± 0.0015. If we use the sampled nuclear data libraries, then we obtain a mean *k*-effective of 0.9718 with a standard deviation of 0.0056 ignoring any uncertainties in manufacturing tolerances

The application case also has some manufacturing tolerances, namely: fuel pellet diameter, cladding inner and outer diameters, active fuel length and the diameters of the inner and outer guide tubes. Again, these are sampled using LHS forming 25 realisations. The application test cases have a MONK category number of either 121 or 157. These categories are for uranium systems with medium non-fuel absorption, medium resonance absorption, low (case 121) to medium leakage (case 157), low fast fission and low fuel hydrogen content. The cases switches between low and medium leakage as they are on the borderline between the two partitions and hence the stochastic differences in the manufacturing tolerances and from the MONK sampling process itself can result in a switch.

Table I contains the basic statistics arising from the nominal case, sampling the nuclear data only, sampling the components (from the manufacturing tolerances) only and from sampling both nuclear data and the components. This table reports the mean, standard deviation, standard error and the mean plus three standard deviations (used frequently as an upper limit in criticality safety calculations). Additionally, the mean plus the 95% confidence interval and the one-tailed upper 95%/95% tolerance limit are also reported. The 95% confidence interval (which is slightly less than two standard deviations) is included in addition to the standard upper bound of three standard deviations as it is a commonly used measure of a confidence interval. The case with sampled components only and the nuclear data only are normally distributed but not the case with both sampled components and sampled nuclear data (using the Shapiro-Wilks test for normality).

**Table I. Basic statistics from application case**

| | Mean | Standard deviation | Mean + 97.5% Confidence Interval | Mean + 3σ | mean plus Upper 95%/95% tolerance limit |
|---|---|---|---|---|---|
| **Nominal case** | 0.9689 | 0.0015 | 0.9718 | 0.9734 | - |
| **Nominal case with nuclear data uncertainties** | 0.9718 | 0.0056 | 0.9829 | 0.9887 | 0.9848 |
| **Sampled components** | 0.9718 | 0.0027 | 0.9771 | 0.9799 | 0.9780 |
| **Sampled components and nuclear data** | 0.9720 | 0.0062 | 0.9842 | 0.9906 | 0.9829 |

## 3.1. Sensitivity Estimation

The manufacturing parameters sensitivities are estimated by least squares fitting using the sampled data only. The method is approximate; however, the results can be used to gauge how sensitive the calculation is to specific parameters. For example, the results in Table II show most sensitivity to the guide tube and cladding diameters. The important data is the order of magnitudes to estimate which components give more sensitivity than others. The sensitivities are only shown for the parameters that are being varied.

**Table II. Estimated sensitivity coefficients**

| | Rank (by magnitude) | Least squares approximation (dimensionless) |
|---|---|---|
| **Guide inner Diameter (cm)** | 1 | -0.2878 |
| **Clad outer diameter (cm)** | 2 | 0.2549 |
| **Guide outer diameter (cm)** | 3 | -0.2465 |
| **Clad inner diameter (cm)** | 4 | -0.2296 |
| **Fuel pellet diameter (cm)** | 5 | 0.1249 |
| **Fuel active length (cm)** | 6 | 0.0631 |

From Table II it can be seen that the guide and cladding diameters are the greatest contributor towards the sensitivities to manufacturing tolerances. The sensitivities were calculated by using standardised variables (which expresses the values in terms of deviations from the mean) so that the magnitudes are not dominant in the calculations. As the diameters of the cladding and guide tubes in addition to the fuel pellets form part of the same fuel pin this might explain the closeness of the magnitudes of the values.

### 3.2. Using the MONK Sensitivity Option

In this subsection we look at the sensitivities due to nuclear data by taking the mean values for the components. We can then use the MONK sensitivity module to estimate the sensitivities to various nuclides and reactions. From Table III, we can see the greatest sensitivities are due to the elastic scatter in the hydrogen within the water reflector and the fission cross section and average number of fissions produced ($\bar{\nu}$) in the U235 within the fuel. These are followed by the oxygen in the water reflector, fission cross section and $\bar{\nu}$ from U238 and the Zirconium in the guide tube.

MONK provides a category number to aid comparisons with ICSBEP and other benchmarks based on partitioning various characteristics of a model, such as resonance absorption, amount of hydrogen in fuel, type of fuel, leakage and fast fission. All of the realisations fall in either Category 109 or 121 in the MONK categorisation system. All of the configurations are Uranium systems with medium non-fuel absorption, low leakage, low fast fission and low fuel hydrogen content. The only difference is in the resonance absorption with some of the cases (e.g. LCT039-10) having medium resonance absorption and some (e.g. LCT039-09) having low resonance absorption. However, the cases are on the borderline between having low resonance absorption and medium resonance absorption in the way that MONK determines the fraction cutoff points. Hence, due to the stochastic nature of the calculation, some cases will fall just within the low resonance absorption range and others in the medium resonance absorption range. This contrasts with the application results given earlier which produced categorisation numbers of 121 or 157.

**Table III. MONK sensitivity results**

| nuclide | Sensitivity (percentage change in K for a 1% change in cross section) | Standard deviation | Uncertainty (%) |
|---|---|---|---|
| U238 nubar (fuel) | 4.1739E-02 | 7.4324E-03 | 6.939E-02 |
| U238 fission (fuel) | 3.4941E-02 | 1.1157E-03 | 8.410E-02 |
| U238 total (fuel) | -6.2886E-02 | 5.7939E-03 | 6.788E-02 |
| U235 nubar (fuel) | 9.8620E-01 | 2.7736E-02 | 6.782E-01 |
| U235 fission (fuel) | 2.7446E-01 | 6.4596E-03 | 1.523E-01 |
| U235 total (fuel) | 1.4273E-01 | 4.6851E-03 | 8.890E-02 |
| O16 total (fuel) | 2.0593E-02 | 4.8718E-03 | 2.536E-02 |
| Fe58 total (guide tube) | 1.8561E-05 | 1.4949E-05 | 2.149E-04 |
| FE57 total (guide tube) | -2.8257E-05 | 1.0839E-05 | 1.363E-03 |
| O16 total (water reflector) | 7.8379E-02 | 6.9964E-03 | 9.651E-02 |
| H1INH2O scatter (water reflector) | 3.3101E-01 | 2.5199E-02 | 2.864E-01 |
| H1INH2O total (water reflector) | 4.6263E-01 | 2.5972E-02 | 4.023E-01 |
| total | | | 9.462E-01 |

### 3.3. Applying Correlations Calculated from ICSBEP Experiments

The International Criticality Safety Benchmark Evaluation Project (ICSBEP) contains many experiments which vary between compositions, geometry, etc. Some of the experiments are similar, and indeed some use the same underlying rigs, fuel, etc in them. Therefore, we can look at the ICSBEP for experiments which are similar to the one described above and see whether they have any uncertainty in their results due to correlations between the integral experiments. Two such experiments are LEU-COMP-THERM-007 (LCT007) and LEU-COMP-THERM-039 (LCT039). In total, we can use 21 different experimental configurations from them to quantify any uncertainties in nuclear data, manufacturing tolerances, number density uncertainties and correlations between the experiments.

Figure 3 shows the correlation matrices when we include geometrical correlations and when we do not. Both correlation matrices include correlations due to nuclear data. As can be seen from figure 3, the correlation matrices are very similar, except that for the LCT007-1 case. Indeed, whether we assume the experiments are correlated or not, the LCT039 cases all demonstrate a strong positive correlation. The nuclear data uncertainties are correlated throughout as the same sampled libraries were used for each experiment and component uncertainty. The assumption of correlations stems from whether the components are assumed to be independent or not. The LCT007 cases (except the first) have a fairly strong negative correlation between the cases. Therefore, we can conclude that there is strong evidence that the cases are correlated.

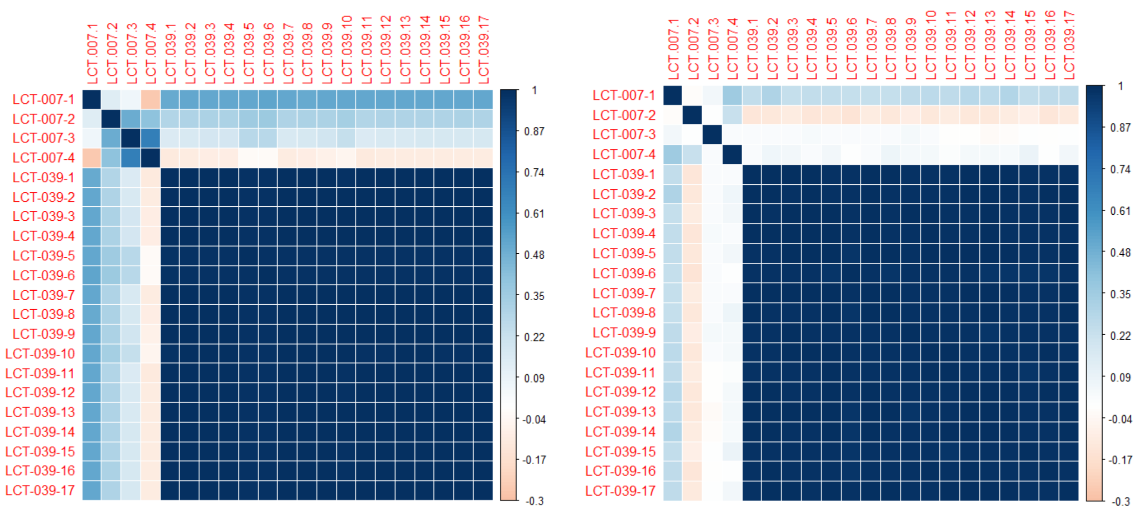


**Figure 3: Correlation matrices with geometric correlations (left) and without (right)**

### 3.4. Statistical Analysis of ICSBEP Experiments

**Table IV. Basic statistics from sampling process for ICSBEP experiments**

| | Nuclear data and manufacturing tolerances | | Manufacturing tolerances only | |
|---|---|---|---|---|
| | **Mean** | **Standard deviation** | **Mean** | **Standard deviation** |
| **Assuming Correlations** | 0.9969 | 0.0176 | 0.9967 | 0.0170 |
| **Assuming no correlations** | 0.9975 | 0.0044 | 0.9972 | 0.0042 |

The above table shows the mean and some basic statistics on the sampled MONK calculations for the experimental benchmarks with similar uncertainty on the estimated bias (with each sample treated independently and no correlations assumed). Table IV also shows the mean estimated bias if we only look at the variation from sampling the manufacturing tolerances. This attempts to remove correlations between the experimental configurations due to nuclear data and manufacturing tolerances when we both assume and not assume common components. It is worth noting that although the results are not normally distributed; if we take the sampled values for each individual configuration (for the mean nuclear data values) the results are normally distributed. The bias can be estimated by using linear regression between a parameter which captures some of the underlying physics of the models. The parameter chosen in this case is that of mean log energy causing fission events. The amount of bias calculated using this method is small which is probably due to the low enriched light water reactor type of system under consideration. We would assume greater biases if we looked at other types of systems such as those with intermediate enriched fuel and non-LWR type assemblies.

**Table V. Application case results including correlations from similar cases**

| | **Assuming no correlations** | | | **Assuming correlations** | | |
|---|---|---|---|---|---|---|
| | **With 97.5% confidence interval from sampling** | **Include three standard deviations** | **Include upper 95%/95% tolerance limit** | **With 97.5% confidence interval from sampling** | **Include three standard deviations** | **Include upper 95%/95% tolerance limit** |
| **Nominal case** | 0.9806 | 0.9852 | 0.9793 | 1.0055 | 1.0233 | 1.0005 |
| **Nominal case with nuclear data uncertainties** | 0.9835 | 0.9881 | 0.9823 | 1.0084 | 1.0262 | 1.0034 |
| **Sampled components** | 0.9835 | 0.9881 | 0.9822 | 1.0084 | 1.0262 | 1.0034 |
| **Sampled components and nuclear data** | 0.9838 | 0.9883 | 0.9825 | 1.0086 | 1.0264 | 1.0036 |

| | **Assuming no correlations** | | | **Assuming correlations** | | |
|---|---|---|---|---|---|---|
| | **Bias from mean log energy causing fission events regression** | **Mean - bias** | **Estimated bias correction using USL method** | **Bias from mean log energy causing fission events regression** | **Mean - bias** | **Estimated bias correction using USL method** |
| **Nominal case** | -0.0087 | 0.9776 | 1.0305 | -0.0090 | 0.9779 | 1.0285 |
| **Nominal case with nuclear data uncertainties** | -0.0085 | 0.9803 | 1.0302 | -0.0087 | 0.9805 | 1.0282 |
| **Sampled components** | -0.0084 | 0.9802 | 1.0303 | -0.0086 | 0.9805 | 1.0284 |
| **Sampled components and nuclear data** | -0.0084 | 0.9804 | 1.0302 | -0.0087 | 0.9807 | 1.0282 |

Table V shows results when we include the uncertainties calculated from the ICSBEP benchmarks with the application case. We also included bounds on that data using the 97.5% confidence interval, the upper 95%/95% tolerance interval and also by adding three standard deviations of the uncertainty from the sampling of the ICSBEP benchmarks as an upper bound (much like traditional criticality safety where $k + 3\sigma$ is taken as an upper limit). Looking at the regression of the multiplication factor against the mean log energy causing fission events then we get a more pessimistic estimate of the bias compared to taking the mean of all of the biases as a constant which is also shown in Table V.

The concept of linear regression may be extended by using the method used to calculate EPD in the MONK validation data base, which is by using the methods of calculating the upper subcritical limit [7].

## 4. CONCLUSIONS

This paper presented a selection of the tools used to estimate errors due to manufacturing tolerances and nuclear data. The work carried out here used the criticality code MONK Version 10A with the JEFF3.1.2 point energy BINGO nuclear data library. The uncertainty quantification methods are associated with the SPRUCE sampling, sampling 25 BINGO libraries (using Latin Hypercube Sampling) and the MONK sensitivity method.

In this paper, taking one representative application, we reported various estimates of the uncertainty in the manufacturing tolerances and nuclear data looking at the mean, mean plus three standard deviations and both the 97.5% confidence interval and the one-sided upper 95%/95% tolerance limit of the application system's multiplication factor. We can draw the following conclusions:

- In our estimates of the sensitivities of the various components in the application case we find that the most sensitive components are the guide tube and clad diameters. This is physically intuitive as we would expect the fuel length and fuel pellet diameter to be the most sensitive out of the list of components with manufacturing tolerances.

- The experimental configurations from the ICSBEP were chosen to be similar to that of the application case, using the MONK classification scheme. The application case is also slightly subcritical compared to that of the configurations to estimate the correlations and their uncertainties. The MONK validation data base can be used to provide a system categorisation to look at similar cases for further analysis if required.

- The data analysis indicates that the correlations in the experimental uncertainties can have a significant effect on the estimated uncertainties for the application calculations. Ignoring the correlations can result in significant underestimation of the uncertainty.

- Estimating correlations in the experimental uncertainties for historic data is a very time-consuming process and success cannot be guaranteed. Therefore ways of avoiding correlated data should be considered, such as the use of a subset of the available experimental data.

The calculations presented in this paper demonstrate the usefulness of tools for uncertainty quantification developed for use with the ANSWERS codes. These can be used to estimate uncertainties arising from nuclear data uncertainties, manufacturing tolerances and modeling uncertainties. Sampling methods are used to estimate total uncertainties, supplemented by sensitivity analysis and response surface fitting to provide factor analysis.

The work detailed in this paper has shown good promise in estimating biases and the powerful use of sampling techniques applied to Monte Carlo criticality codes. However, these methods may be improved in the future to obtain better estimates to the various sensitivities by using variance based sensitivity analysis (such as Sobol indices) and through the use of non-intrusive Polynomial Chaos. Additionally, it would be useful in the future to take into account the methods used to improve the validation of criticality safety codes and the errors in physical data used to ensure that criticality calculations remain within safety limits. Improvements to the calculated bias may also be achieved by using Bayesian statistics where we can use the benchmark data as the a priori information and (assuming a Gaussian distribution) use this to correct for biases assumed in the application model.

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