Development of Benchmark Experiment Sets Applicable to Thorium-Fueled Power Reactor Bias-Calculations

S. Langton and A. Buijs
McMaster University, Engineering Physics, Ontario, Canada
langtose@mcmaster.ca

Abstract

A technique for developing sets of benchmark experiments that are applicable to power reactor bias calculations has been analyzed. A set of potential ZED-2 critical facility experiments was designed such that they could be used in establishing the code biases of three power reactor designs: a CANDU-type reactor with 37-element $(Th,Pu)O_2$ fuel bundles, a CANDU-type reactor with 43-element $(Th,Pu)O_2$ fuel bundles, and a Canadian supercritical water reactor design. Possible ZED-2 experimental arrangements were modified in order to develop a single set of six potential experiments for which the total relative power reactor sensitivity coverage for each power reactor was 0.7 or greater.

1. Introduction

When using reactor physics simulations to model the response of a reactor core, certain limitations are encountered affecting the accuracy of the results. One such limitation results from uncertainties in the tabulated nuclear data used in the simulations. These uncertainties (in the form of variances and covariances) propagate to the resulting calculated multiplication factor. The result is that there is a bias (absolute difference) between the calculated multiplication factor and the multiplication factor that would be found if an exact replicating experiment were to be performed. The determination of this bias is required in order to validate the calculation method being used.

One of the methods that can be used to determine the bias is a generalized linear least squares adjustment procedure [1] which requires the use of a set of experiments. This procedure adjusts the nuclear data and experiment multiplication factors within their uncertainties in order to decrease the biases between experiment simulations and experiment results. The adjusted nuclear data is then applied to a power reactor design. The difference in result between the adjusted and the un-adjusted calculations is a measure of the bias. In order to ensure that a set of experiments is applicable to the bias calculation of a particular power reactor, similarity parameters can be analysed which examine the sensitivities and uncertainties of the experiments and the application. The main similarity parameter used here as a metric for applicable experiments is known as the completeness and represents the relative power reactor sensitivity coverage. The similarity index c_k, representing the similarity of uncertainties, is also briefly examined.

In this paper we describe a set of potential benchmark experiments that has been developed for the ZED-2 heavy-water critical facility at the Chalk River Laboratories. The set has been designed such that together the experiments allow for a high completeness parameter when applied to three separate reactor designs. The designs are a CANDU-type reactor with 37-element $(Th,Pu)O_2$ fuel bundles, a CANDU-type reactor with 43-element $(Th,Pu)O_2$ fuel bundles, and a recent Canadian supercritical water reactor (SCWR) design [2] with 78-element fuel assemblies [3]. Simulations for these purposes were performed using modules of the SCALE 6.1 code package provided by RSICC [4]. In particular, the sensitivity and uncertainty analysis TSUNAMI modules were used.

2. Theory overview

When developing a benchmark set of experiments, the quantities of interest are the nuclear data sensitivities, the nuclear data uncertainties, and (based on the aforementioned) the similarity parameters. These values are described in the following sections.

2.1 Sensitivities

Sensitivities are a representation of the change in a parameter such as the multiplication factor k with a small change in a particular cross section. For example, the relative explicit sensitivity $S_{k,\Sigma(r)}$ of a cross section Σ at position r is [6]:

$$\frac{\Delta\Sigma(r)}{\Sigma(r)} S_{k,\Sigma(r)} = \frac{\Delta \mathrm{k}}{\mathrm{k}} \tag{1}$$

This can be transformed using partial derivatives to define the relative explicit sensitivity coefficient as:

$$S_{k,\Sigma(r)} \equiv \frac{\Sigma(\mathrm{r})}{\mathrm{k}} \frac{\partial \mathrm{k}}{\partial \Sigma(\mathrm{r})} \tag{2}$$

To calculate the total relative sensitivity, an implicit component that accounts for changes in the multiplication factor due to resonance self-shielding cross section adjustments is added to the explicit component. These sensitivities are computed using the SAMS module of the SCALE 6.1 code package [5].

2.2 Similarity parameters

Based on the sensitivities, parameters can be defined which quantify the similarity between systems. There are a number of possible similarity parameters, however the focus here is on the similarity integral index c_k and the completeness R.

2.1.1 Integral index c_k

The integral index c_k is a representation of the similarity in the uncertainties of the cross section data (variances and covariances) of two systems (i.e. an experiment and an application such as a power reactor). [6]

Let $\boldsymbol{\alpha}=\alpha_m$, $m=1,2,\ldots,M$ represent a matrix containing the nuclear data, where M is a product of the number of nuclide-reaction pairs with the number of energy groups. An $M\times M$ matrix containing the relative variances and covariances is then:

$$C_{\alpha,\alpha} = \frac{COV(\alpha_m, \alpha_p)}{\alpha_m \alpha_p}, m = 1,2,\ldots,M, p = 1,2,\ldots,M \tag{3}$$

Where COV indicates the covariance. An $I \times I$ matrix C_{kk} representing the uncertainties (variances and covariances) between I systems can then be found as:

$$C_{kk} = S_k C_{\alpha\alpha} S_k^{\dagger} \tag{4}$$

Where S_k is an $I\times M$ matrix containing sensitivities. The correlation coefficient c_k between two of the systems considered, i and j is then the ratio of the covariance to the product of the standard deviation of each.

$$c_k = \frac{\sigma_{ij}^2}{\sigma_i \sigma_j} \tag{5}$$

2.1.2 Completeness

The completeness parameter R is a measure of how well the sensitivities of a set of experiments cover the sensitivities of an application. [6]

$$R = \frac{S_a}{S_t} \tag{6}$$

$$S_a = \sum_n \sum_x \sum_j |dS_{x,j}^{a,n}| \tag{7}$$

$$S_t = \sum_n \sum_x \sum_j |S_{x,j}^{a,n}| \tag{8}$$

$$d = \begin{cases} 1\ if\ N_{x,j}^n \geq nixlim \\ 0\ if\ N_{x,j}^n < nixlim \end{cases} \tag{9}$$

$$N_{x,j}^n = number\ of\ experiments\ where\ \left|S_{x,j}^{e,n}\right| > |senfac \times S_{x,j}^{a,n}| \tag{10}$$

Where a is the application, n is the nuclide, x is the reaction, j is the energy group, N is the number of systems where the magnitude of the sensitivity of the experiment is greater than that of the application multiplied by the factor *senfac* (here this is 0.9), and *nixlim* is the minimum number of experiments with a sensitivity greater than that of the application for the application's sensitivity to be considered covered.

In essence, the completeness is a representation of how well the cross section sensitivities of the application are being covered by the experiments, where a 'covered' sensitivity means the experiment sensitivity is higher than that of the application. It is desirable to ensure the experiment sensitivities are larger because cross sections sensitivities are a representation of the 'importance' of a cross section as it pertains to the calculation of the multiplication factor. A high sensitivity means that when performing a bias adjustment procedure in which the cross sections are being adjusted, a relatively small change to that cross section would result in a large change to the multiplication factor. The goal of having experiments with sensitivities larger than those of the application is to ensure the importance of each cross section to the application is not underestimated.

The development of a benchmark experiment set that would offer an adequate completeness has been the focus of this analysis. The limitation for an adequate completeness value that was used here was 0.7 or greater [7].

3. Sensitivity analysis

To design a benchmark set of experiments with a high completeness, it is important to first analyse the sensitivities of the applications of interest. Larger sensitivities are weighted higher in the completeness formula so these sensitivities are the most important to cover. Knowing which isotopes have the largest sensitivities allows for better experiment design choices.

For the sensitivity analysis, as well as the subsequent similarity study, KENO models of each of the power reactor designs were developed using a 238- group cross section library (KENO being a Monte Carlo transport solver module of the SCALE 6.1 code package). The CANDU-type cores were modelled as snapshots of time-average cores. The SCWR was modelled at averaged beginning of cycle (BOC) and end of cycle (EOC) states. These were then used in the TSUNAMI modules to calculate sensitivities and uncertainties.

Tables 1-4 indicate the nuclide/reaction pairs with the five largest sensitivities for each power reactor.

Table 1 CANDU (37-element) Largest sensitivities.

Nuclide/Reaction Pair	Sensitivity
Pu-239 $\bar{\nu}$	0.83
Pu-239 fission	0.48
Th-232 (n,γ)	-0.33
Pu-239 (n,γ)	-0.17
Pu-241 $\bar{\nu}$	0.09

Table 2 CANDU (43-element) Largest sensitivities.

Nuclide/Reaction Pair	Sensitivity
Pu-239 $\bar{\nu}$	0.83
Pu-239 fission	0.48
Th-232 (n,γ)	-0.34
Pu-239 (n,γ)	-0.17
Pu-241 $\bar{\nu}$	0.09

Table 3 SCWR (BOC) Largest sensitivities.

Nuclide/Reaction Pair	Sensitivity
Pu-239 $\bar{\nu}$	0.60
Pu-241 $\bar{\nu}$	0.31
Pu-239 fission	0.30
Pu-241 fission	0.16
Pu-239 (n,γ)	-0.16

Table 4 SCWR (EOC) Largest sensitivities.

Nuclide/Reaction Pair	Sensitivity
Pu-239 $\bar{\nu}$	0.50
Pu-241 $\bar{\nu}$	0.32
Pu-239 fission	0.27
Pu-241 fission	0.18
Th-232 (n,γ)	-0.15

The highest sensitivities for all of the power reactor designs tend to be to Pu-239 and Pu-241 isotopes. It is therefore necessary to make the coverage of these sensitivities a focus when developing the benchmark experiment set.

4. Benchmark set development

To develop a set of experiments that together achieve a high completeness, there are two main focuses. The first is to ensure that isotopes for which the power reactor designs have a high sensitivity are present in the core in sufficient quantity. If the isotope is only present in very small quantities (or of course if it is not present at all) then it will likely not have a high enough sensitivity to cover the application sensitivity. The second focus is on the energy of the neutrons in the core. If there are more high energy neutrons, then high energy cross sections tend to be covered, and vice versa. Thus, when designing a benchmark set, it is important to examine the energy spectrum of uncovered sensitivities of the power reactor, and note which modifications to the test reactor core tend to cover these energy ranges. For example, if the fuelled channels are very close together, there tend to be more high energy neutrons in the core, so the high energy sensitivities are larger, whereas if they are farther apart there are more thermal energy neutrons.

For the experiments designed here, modifications were made to the following parameters of the ZED-2 critical facility experiments: the fuel type, the lattice arrangement, the lattice pitch and the coolant type. By modifying these values, the experiments were deliberately designed such that the highest sensitivities were covered. In an attempt to develop realistic experiments, a set of five limiting conditions for safe operation (LCO) for the ZED-2 critical facility were used as guidelines.

To build a set of applicable experiments, an iterative approach was taken wherein after each new potential experiment was simulated the completeness with this new addition was analysed, along with the largest uncovered sensitivities, and the sensitivity spectrum of a user-defined nuclide of interest. Not all of this information was explicitly available from the TSUNAMI modules. Thus, a separate script analysing the sensitivity data files was written for the purpose.

4.1 Final benchmark set

For the final set of benchmark experiments, three fuel types were chosen. These are the fuel used in the CANDU-type reactor designs, and two modified versions of the fuel used in the SCWR. The reason two fuel types were used to represent the SCWR fuel is that the proposed SCWR fuel has a high plutonium content at 13 wt%. Using this fuel type, the safety limits of the ZED-2 critical facility could not be met while at the same time an experiment useful to the current study was created. Thus, two fuel types with lower plutonium content were used. The fuel compositions are listed in Table 5. Note that for the current study the availability and expense of these fuel types at the ZED-2 facility was not a considered factor.

Table 5 Experiment set fuel compositions.

	Fuel 1	Fuel 2	Fuel 3
Nuclide	wt%	wt%	wt%
Th-232	86.051	85.682	81.727
Pu-238	0.002	0.061	0.169
Pu-239	1.181	1.146	3.209
Pu-240	0.303	0.506	1.418
Pu-241	0.045	0.336	0.941
Pu-242	0.008	0.157	0.438
O-16	12.410	12.113	12.097

Figure 1 shows the ZED-2 lattice arrangement used in the experiments (view from above).

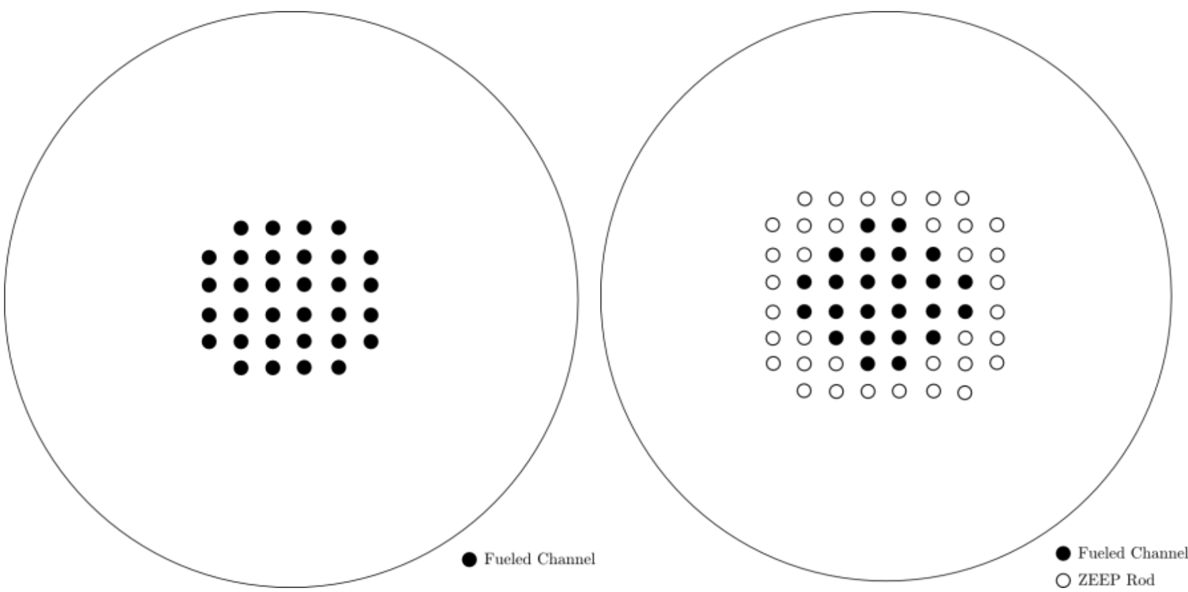

Figure 1 ZED-2 Lattice arrangements (Geometry 1 (left), Geometry 2 (right))

Table 6 describes the benchmark experiments chosen, along with the important of each added experiment with respect to the sensitivity regions it tends to cover.

Table 6 Experiment set.

Exp #	Fuel	Fuelled Channels	Coolant	Pitch	Importance
1	Type 1	32 (Geometry 1)	H_2O	14.0 cm	Pu-239 fission low energy
2	Type 1	32 (Geometry 1)	D_2O	38.0 cm	Pu-239 fission high energy
3	Type 1	32 (Geometry 1)	Air	38.0 cm	Th-232 capture
4	Type 2	32 (Geometry 1)	H_2O	28.0 cm	Pu-241 fission low energy
5	Type 2	24 and 36 ZEEP (Geometry 2)	Air	20.0 cm	Pu-241 fission low energy
6	Type 3	32 (Geometry 1)	D_2O	13.0 cm	Pu-241 fission high energy

The estimated LCOs of these experiments are listed in Table 7 and 8, where H_c is the critical moderator height, P_A is the actual power at an indicated power of 200 W, M_f is the mass of heavy elements in the fuel that is submerged, t_{gen} is the generation time, and LCR_c is the corrected level coefficient of reactivity [8]. To perform these experiments, further safety concerns would likely need to be addressed that have not been considered here.

Table 7 Experiment LCOs (Part 1)

Parameter	Limit	Experiment 1	Experiment 2	Experiment 3
H_c (cm)	≤265	176	175	219
P_A (W)	≤700	612±4	449±1	613±3
M_f (kg)	>1740	1768	1760	2244
t_{gen} (ms)	>0.25	0.3544±0.0007	1.4489±0.0004	1.4636±0.0005
LCR_c (mk/cm)	$0.12 \leq LCR_c \leq 2.25$	0.4±0.1	1.0±0.1	0.8±0.1

Table 7 Experiment LCOs (Part 2)

Parameter	Limit	Experiment 4	Experiment 5	Experiment 6
H_c (cm)	≤265	196	150	200
P_A (W)	≤700	580±3	365±2	421±1
M_f (kg)	>1740	2087	1936	2133
t_{gen} (ms)	>0.25	1.3535±0.0007	0.7317±0.0006	0.737±0.001
LCR_c (mk/cm)	$0.12 \leq LCR_c \leq 2.25$	0.6±0.1	0.9±0.1	0.2±0.1

Using these experiments for all of the power reactors being examined here, the following completeness values result.

Table 8 Completeness results.

Application	Completeness
CANDU (37-element)	0.76
CANDU (43-element)	0.75
SCWR (BOC)	0.77
SCWR (EOC)	0.70

Thus using the same set of six experiments, the completeness for all of the power reactors analysed is above the 0.7 completeness limit, assuming only one experiment must cover the sensitivity for the sensitivity to be considered covered. The coverage of some of the largest sensitivities is shown in Figures 2-5. In the figures, the 'Experiments' plots represent the combination of the maximum sensitivities from all of the experiments together. These have been overlaid on the application sensitivities in order to show the coverage. For clarity, an outline of the application sensitivities is shown on the figure so that in cases of full coverage the difference between the application and experiments sensitivities are clear.

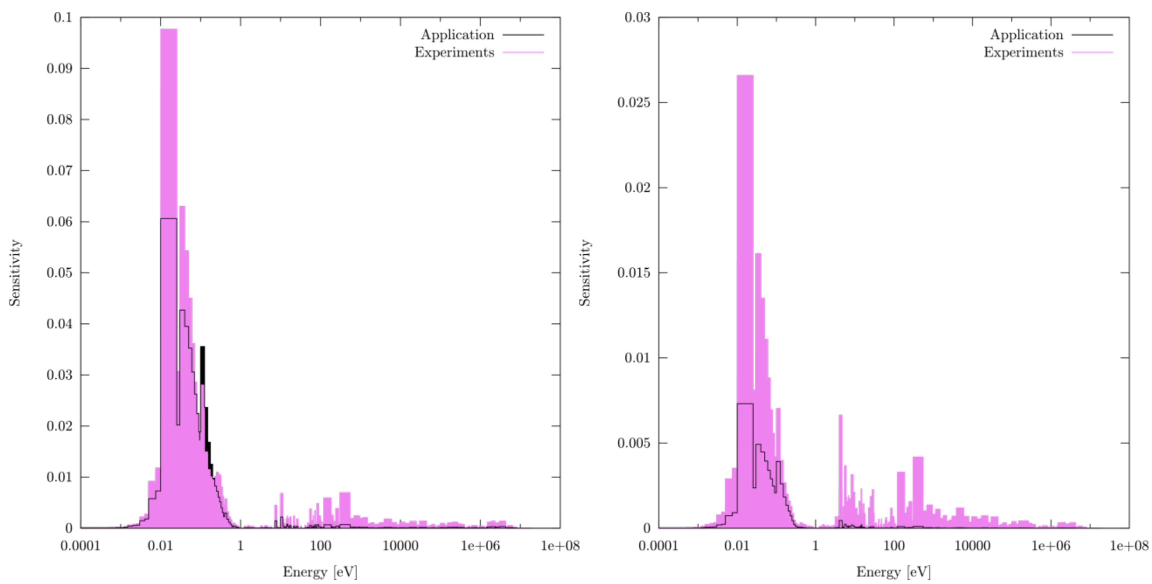

Figure 2 CANDU (37-el) Coverage of Pu-239 (left) and Pu-241 (right) fission sensitivities.

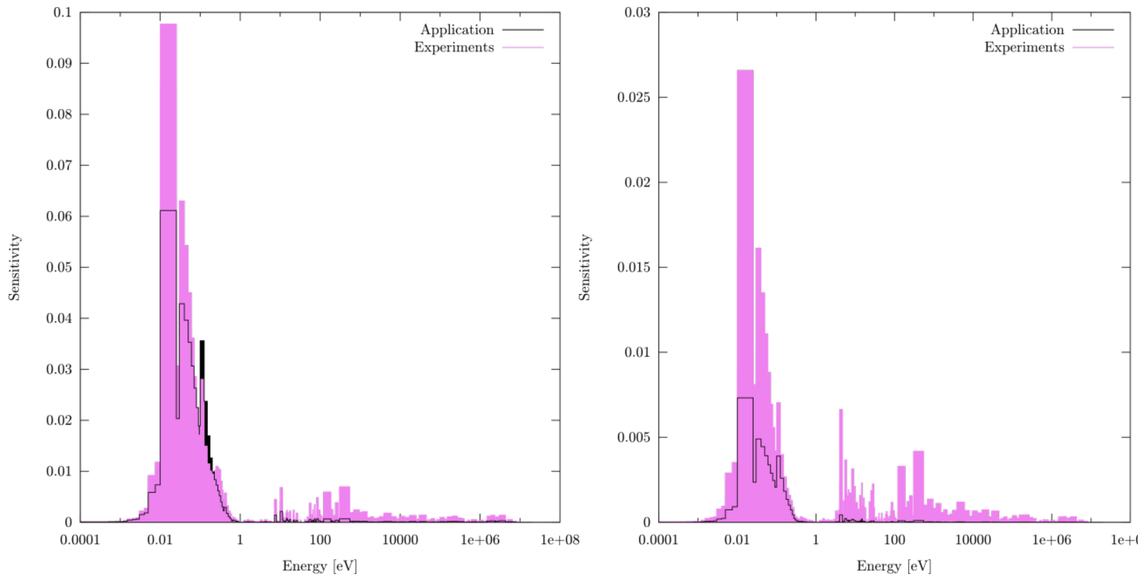

Figure 3 CANDU (43-el) Coverage of Pu-239 (left) and Pu-241 (right) fission sensitivities.

The results show that for the CANDU-type reactors, the experiment set provides full coverage of the Pu-241 fission cross section sensitivities listed. The Pu-239 cross section sensitivities are covered in low and high energy regions, however they are not covered in a range near 0.1 eV.

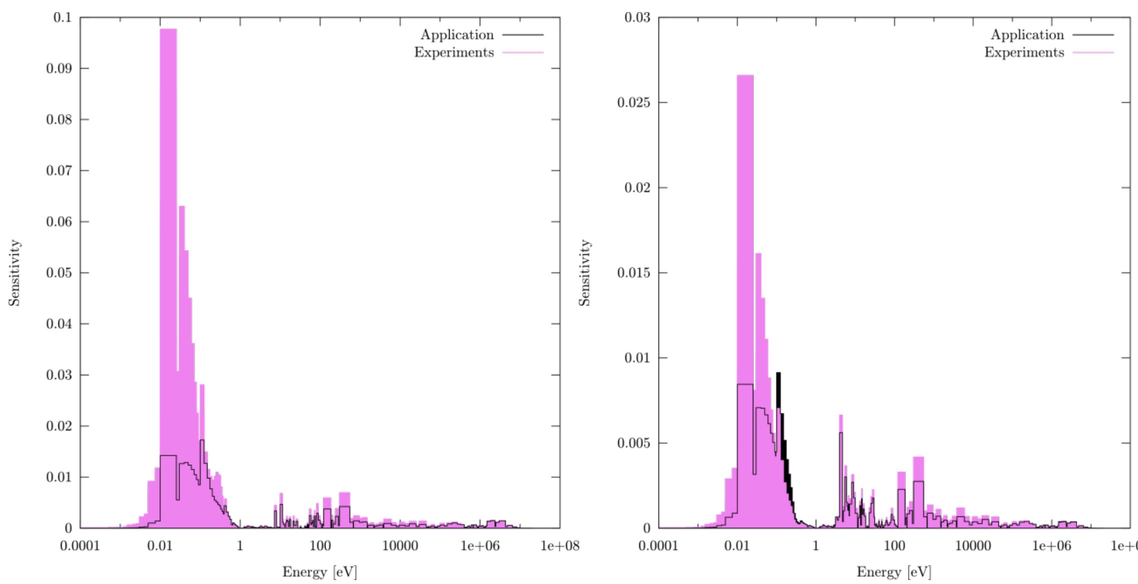

Figure 4 SCWR (BOC) Coverage of Pu-239 (left) and Pu-241 (right) fission sensitivities.

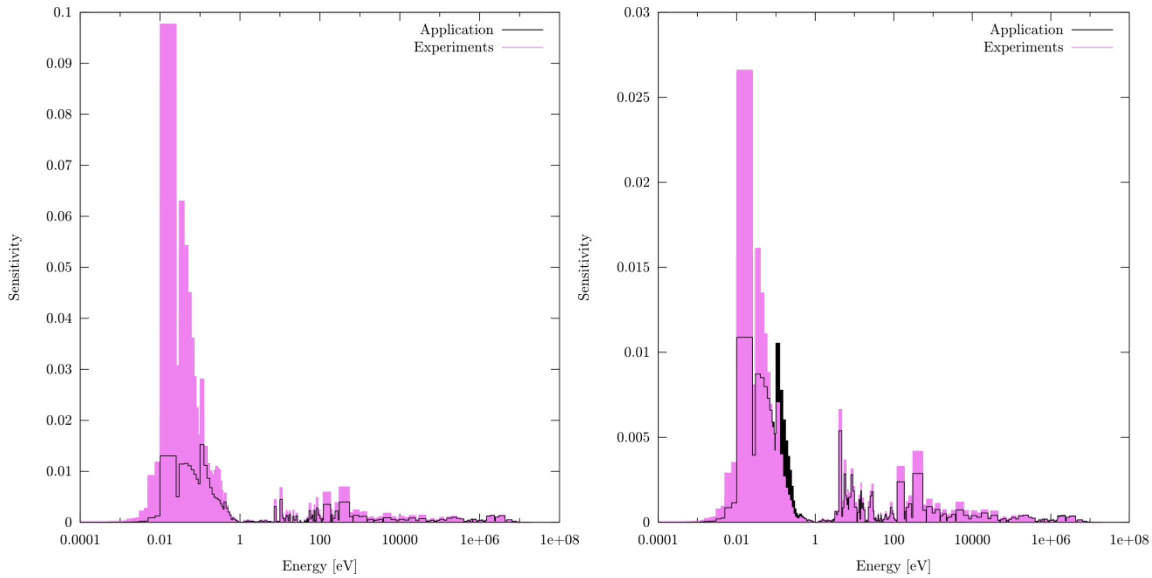

Figure 5 SCWR (EOC) Coverage of Pu-239 (left) and Pu-241 (right) fission sensitivities.

For the BOC and EOC SCWR cases, the Pu-239 cross section sensitivities are fully covered while the Pu-241 sensitivities are not. Again, the uncovered sensitivities are at energies of approximately 0.1 eV. This indicates that for future additions to the experiment set, focusing on the 0.1 eV energy range would be useful to increase the cross section sensitivity coverage.

The five largest uncovered sensitivities after applying the experiment sets are shown in Tables 10-12 for each power reactor.

Table 9 CANDU (37-element) Largest uncovered sensitivities.

Nuclide/Reaction Pair	Sensitivity
Pu-239 $\bar{\nu}$	0.16
Pu-239 fission	0.09
Th-232 (n,γ)	-0.08
U-233 $\bar{\nu}$	0.07
Pu-239 (n,γ)	-0.04

Table 10 CANDU (43-element) Largest uncovered sensitivities.

Nuclide/Reaction Pair	Sensitivity
Pu-239 $\bar{\nu}$	0.16
Pu-239 fission	0.09
Th-232 (n,γ)	-0.08
U-233 $\bar{\nu}$	0.07
Pu-239 (n,γ)	-0.04

Table 11 SCWR (BOC) Largest uncovered sensitivities.

Nuclide/Reaction Pair	Sensitivity
Pu-241 $\bar{\nu}$	0.09
U-233 $\bar{\nu}$	0.06
Pu-241 fission	0.04
Pu-240 (n,γ)	0.03
U-233 fission	-0.03

Table 12 SCWR (EOC) Largest uncovered sensitivities.

Nuclide/Reaction Pair	Sensitivity
U-233 $\bar{\nu}$	0.13
Pu-241 $\bar{\nu}$	0.10
U-233 fission	0.07
Pu-241 fission	0.05
Pu-240 (n,γ)	-0.04

The largest uncovered sensitivities still tend to belong to Pu-239, Pu-240, U-233 isotopes present in the fuel. However, the Th-232 and U-233 sensitivities are now of more significance and to further increase the completeness, the sensitivities of these isotopes could be a focus.

As was mentioned above, for the study performed here it was assumed that only one experiment must have a sensitivity greater than that of the application in order for it to be considered covered. In general it would be advisable to have more experiments covering each sensitivity. This is because when performing a GLLS adjustment in which the cross sections are being modified it is not advisable to have the adjustment of each cross section based solely on one experiment. For the set developed here, however, the similarity in the geometry and materials used in the experiments mean the similarity index c_k both between the experiments and between the experiments and the applications is high (0.76-1.0). This index represents the similarity of the uncertainties in the nuclear data. This indicates that changes to important cross sections in one experiment would also tend to affect the other experiments (although perhaps to a lesser degree due to a smaller sensitivity). This makes the use of only a small number of experiments reasonable for the current study. An analysis of the number of experiments covering each sensitivity, and the value of a high similarity between experiments, would be useful, and the addition of further experiments (either newly designed experiments or existing experiments) may still be advisable. Tables 13 and 14 indicate the similarity indices c_k for each case.

Table 13 Similarity between experiments.

Exp #	1	2	3	4	5	6
1	-------	0.97	0.89	0.96	0.82	0.88
2	0.97	-------	0.92	0.97	0.85	0.85
3	0.89	0.92	-------	0.94	0.92	0.86
4	0.96	0.97	0.94	-------	0.90	0.88
5	0.82	0.85	0.92	0.90	-------	0.89
6	0.88	0.85	0.86	0.88	0.89	-------

Table 14 Similarity between experiments and applications.

Exp #	CANDU (37)	CANDU (43)	SCWR (BOC)	SCWR (EOC)
1	0.88	0.88	0.80	0.76
2	0.89	0.89	0.79	0.76
3	0.97	0.97	0.85	0.81
4	0.96	0.92	0.85	0.82
5	0.89	0.89	0.88	0.86
6	0.84	0.84	0.89	0.87

The completeness parameter calculated here only considers the sensitivities of the nuclear data. However, it may be useful to consider weighting the sensitivities in this formula by the uncertainties in the cross sections. This is because the GLLS method adjusts the cross sections such that they remain within their uncertainty range. Thus, if an application has a cross section with a small sensitivity but a large uncertainty, the importance of this cross section to the adjustment procedure may be underestimated. Further analysis of this hypothesis is necessary.

5. Conclusions

Using sensitivity analysis techniques, a similarity study was performed in order to develop a set of experiments that would be applicable to a generalized linear least squares adjustment for a CANDU-type reactor design with 37-element $(Th,Pu)O_2$ fuel bundles, a CANDU-type reactor design with 43-element $(Th,Pu)O_2$ fuel bundles, and an SCWR design (BOC and EOC). The experiments were designed such that together they achieved a high completeness, an indicator of cross section sensitivity coverage.

Using one set of six potential experiments for the ZED-2 critical facility, a completeness greater than 0.7 was achieved for all of the power reactors analysed. These experiments were designed specifically such that they would be useful for this analysis. A completeness in this range indicates that the experiments would be useful in the determination of the bias in the power reactor multiplication factor, which is necessary when performing safety analyses. This analysis exemplifies the value in designing experiments particularly for the purposes of adjustment procedures and bias determinations.

Here the experiment was designed such that only one experiment must have a completeness greater than that of the application to be considered covered. This is reasonable due to the high similarity index c_k between the experiments. However, it would be useful to design more experiments to cover each sensitivity or alternatively to choose existing experimental data that is applicable to the similarity study.

6. References

[1] B. Broadhead, C. Hopper, *et al.*, "Criticality safety applications of S/U validation methods", Proceedings of the ANS/ENS 2000 International Winter Meeting and Embedded Topical Meetings, Washington DC, USA, 2000 November.

[2] L. K. H. Leung, *et al.*, "A next generation heavy water nuclear reactor with supercritical water as coolant", Proceedings of the International Conference on the Future of HWRs, Ottawa, Ontario, Canada, 2011 October 2-5.

[3] J. Pencer, "SCWR 78-element bundle reference model", Tech. Rep. 217-123700-REPT-001, Atomic Energy of Canada Limited, 2011 September.

[4] Radiation Safety Information Computational Center, Oak Ridge National Laboratory, http://rsicc.ornl.gov, 2013.

[5] B. T. Rearden, *et al.*, "SAMS: Sensitivity analysis modules for SCALE", Tech. Rep. ORNL/TM-2005/39 Version 6.1 Sect. F22, Oak Ridge National Laboratory, 2011 June.

[6] B. T. Rearden and M. A. Jessee, "TSUNAMI utility modules", Tech. Rep. ORNL/TM-2005/39 Version 6.1 Sect. M18, Oak Ridge National Laboratory, 2011 June.

[7] M. L. Williams *et al.*, "TSURFER: An adjustment code to determine biases and uncertainties in nuclear system responses by consolidating differential data and benchmark integral experiments", Tech. Rep. ORNL/TM-2005/39 Version 6.1 Sect. M21, Oak Ridge National Laboratory, 2011 June.

[8] G. B. Wilkin, "ZED-2 reactor capabilities and the new license safety case", Proceedings of the ZED-2 Winter School, Chalk River, Ontario, Canada, 2011 December.