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On the use of integral experiments for uncertainty reduction of reactor macroscopic parameters within the TMC methodology



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ABSTRACT

The current nuclear data uncertainties observed in reactor safety parameters for some nuclides call for safety concerns especially with respect to the design of GEN-IV reactors and must therefore be reduced significantly. In this work, uncertainty reduction using criticality benchmark experiments within the Total Monte Carlo methodology is presented. Random nuclear data libraries generated are processed and used to analyze a set of criticality benchmarks. Since the calculated results for each random nuclear data used are different, an algorithm was used to select (or assign weights to) the libraries which give a good description of experimental data for the analyses of the benchmarks. The selected or weighted libraries were then used to analyze the ELECTRA reactor. By using random nuclear data libraries constrained with only differential experimental data as our prior, the uncertainties observed were further reduced by constraining the files with integral experimental data to obtain a posteriori uncertainties on the $k_{\rm eff}$. Two approaches are presented and compared: a binary accept/reject and a method of assigning file weights based on the likelihood function. Significant reductions in ²³⁹Pu and ²⁰⁸Pb nuclear data uncertainties in the $k_{\rm eff}$ were observed after implementing the two methods with some criticality benchmarks for the ELECTRA reactor.

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1. Introduction

To fulfill target accuracies for GEN-IV systems (Salvatores et al., 2008), the current nuclear data uncertainties observed in reactor safety parameters for some nuclides would have to be reduced significantly. Reduction of nuclear data uncertainties using differential experimental data within the Total Monte Carlo (TMC) methodology (Koning and Rochman, 2008) has been investigated by several authors. First, we recall the so-called 'Filtered Monte Carlo' proposed in Smith (2004) and implemented at Nuclear Research and Consultancy Group (NRG), Petten (Koning and Rochman, 2012) where nuclear model parameter uncertainties are predetermined after comparison with existing experimental uncertainties. By varying model parameters within these experimental uncertainties, a full covariance matrix is obtained which

include off-diagonal correlations (Bauge et al., 2010). In Duan et al. (2014), model calculations within the TMC methodology were compared with experimental data by computing a weighted χ^2 for each reaction channel. Large weights were assigned to reactions with a large number of experimental data, to channels with more precise data, and to large cross sections. In Helgesson et al. (2015), Koning, (2015), file weights proportional to the likelihood function are assigned to TENDL random files based on their comparison with differential experimental data. By computing a generalized χ^2 , experimental uncertainties and their correlations are included.

Even though information from differential measurements together with their uncertainties are included in the TMC methodology, wide spreads have been observed in the parameter distributions leading to large uncertainties in reactor parameters for some nuclides for the European Lead-Cooled Training Reactor (Alhassan et al., 2014a, 2013, 2015a, 2014b). Due to safety concerns and the development of GEN-IV reactors with their challenging technological goals (GIF, 2014), these uncertainties should be



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reduced significantly. In Alhassan et al. (2014a), an accept/reject method was proposed for uncertainty reduction using arbitrary χ^2 limits as constraints for accepting random nuclear data files based on integral benchmark information. The method was applied to reactor burnup calculations for the European Lead-Cooled Training Reactor (ELECTRA) (Sjöstrand et al., 2014). In Alhassan et al. (2014b), the method was improved by including benchmark uncertainty information and a method of assigning file weights was also proposed. In Rochman et al. (2014), an approach for improving neutronics simulations using a linear combination of nuclear data files and weights based on integral benchmarks was investigated. In the study, the χ^2 estimator was used to compare the performance of random nuclear data files using a series of nuclear data libraries as the reference library. By using this method, a set of 'best' random files with better C/E values were selected in combination with each nuclear data library (Rochman et al., 2014). Also, some works on the methods and issues for the combined use of integral experiments and covariance data have been carried out by subgroup 33 of the Organisation for Economic Co-operation and Development (OECD), Nuclear Energy Agency's Nuclear Science Committee (Salvatores et al., 2013).

In this work, a comparison between a binary accept/reject and a method of assigning file weights in uncertainty reduction calculations using a set of criticality experiments within the TMC methodology is presented for the ELECTRA reactor. Random nuclear data libraries produced using the TALYS based system are processed and used to analyze a set of benchmarks. Since the calculated results are different for each random nuclear data library used, we use an algorithm to select (or assign weights to) those libraries which give a good description of experimental data for the analyses of the benchmarks. With the selected or weighted libraries, the ELECTRA reactor was analyzed. The result is that the uncertainty margins on ELECTRA are reduced. By using random nuclear data files constrained with only differential experiments as our prior, the uncertainties observed were further reduced by using integral experimental data as an additional constraint to obtain a posteriori uncertainties in the $k_{\rm eff}$. Also, since integral experiments normally contain different isotopes, this complicates the use of these experiments for nuclear data uncertainty reduction. This complication is particularly addressed in this work.

2. Reactor description

The European Lead-Cooled Training Reactor (ELECTRA) is a conceptual 0.5 MW lead cooled reactor fueled with (Pu,Zr)N with an estimated average neutron flux at beginning of life of 6.3×10^{13} n/cm² s (Wallenius et al., 2012). The fuel composition is made up of 60% mol of ZrN and 40% mol of PuN. ELECTRA is cooled by pure lead. The objective is to achieve a 100% heat removal via natural convection while ensuring enough power density to keep the coolant in a liquid state. The core is hexagonally shaped with an active core height of 30 cm and consists of 397 fuel rods. Reactivity compensation is achieved by the rotation of absorbing drums made up of B_4C enriched to 90% in B10, having a pellet density of 2.2 g/ cm³ (Wallenius et al., 2012). A detailed description of the reactor is presented in Wallenius et al. (2012).

3. Benchmark cases

The benchmarks used in this work were obtained from the International Criticality Safety Benchmark Evaluation Project (ICS-BEP) (International Handbook of evaluated Criticality Safety Benchmark Experiments, 2011). In the ICSBEP handbook, benchmarks experiments are categorized according to their fissile media (Plutonium, highly enriched uranium (HEU), low-enriched uranium (LEU) etc.), their physical form (metal, compound, solution etc.), their neutron energy spectrum (thermal, intermediate, fast and mixed spectra) and a three digit reference number. In this work, four types of benchmarks were used: PU-MET-FAST (Plutonium Metallic Fast), PU-MET-INTER (Plutonium Metallic Intermediate), HEU-MET-FAST (Highly enriched uranium Metallic Fast) and LEU-COMP-THERM (Low-enriched uranium Compound Thermal) systems. The benchmarks, the evaluated benchmark uncertainties, their case numbers together with the isotopes varied under each case are presented in Table 1.

4. Methodology

To accomplish our goal of further reducing nuclear data uncertainties, we use criticality benchmark experimental information as an additional constraint in the TMC methodology as presented in

Table 1

Criticality safety benchmarks used in this work with their case numbers, the evaluated Benchmark k_{eff} , the evaluated benchmark uncertainty and the isotopes varied in the TMC method (Each isotope was varied one after the other). These benchmarks were obtained from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) (International Handbook of evaluated Criticality Safety Benchmark Experiments, 2011). PU-MET-FAST stands for Plutonium Metallic Fast, PU-MET-INTER for Plutonium Metallic Intermediate, HEU-MET-FAST for Highly Enriched Uranium (HEU) Metallic Fast and LEU-COMP-THERM for Low Enriched Uranium (LEU) Compound Thermal benchmarks.

Benchmark category	Case	Evaluated benchmark $k_{\rm eff}$	Evaluated benchmark uncertainty [pcm]	Varied isotopes
PU-MET-FAST-001	1	1.000	200	^{239,240,241} Pu
PU-MET-FAST-002	1	1.000	200	^{239,240,241} Pu
PU-MET-FAST-005	1	1.0000	130	^{239,240,241} Pu
PU-MET-FAST-008	1	1.000	60	^{239,240,241} Pu
PU-MET-FAST-009	1	1.0000	270	^{239,240,241} Pu
PU-MET-FAST-010	1	1.0000	180	^{239,240,241} Pu
PU-MET-FAST-011	1	1.000	100	^{239,240,241} Pu
PU-MET-FAST-012	1	1.0009	100	^{239,240,241} Pu
PU-MET-FAST-013	1	1.0034	100	^{239,240,241} Pu
PU-MET-FAST-035	1	1.0000	160	^{206,207,208} Pb, ^{239,240} Pu
PU-MET-INTER-002	1	0.9862	50	^{239,240,241} Pu
HEU-MET-FAST-027	1	1.0000	250	^{206,207,208} Pb, ^{235,238} U
HEU-MET-FAST-057	1	1.0000	200	^{206,207,208} Pb, ^{235,238} U
HEU-MET-FAST-057	2	1.0000	230	^{206,207,208} Pb, ^{235,238} U
HEU-MET-FAST-057	3	1.0000	320	^{206,207,208} Pb, ^{235,238} U
HEU-MET-FAST-057	4	1.0000	400	^{206,207,208} Pb, ^{235,238} U
HEU-MET-FAST-057	5	1.0000	190	^{206,207,208} Pb, ^{235,238} U
HEU-MET-FAST-064	1	0.9996	80	^{206,207,208} Pb, ^{235,238} U
LEU-COMP-THERM-010	21	1.0000	210	^{206,207,208} Pb, ^{235,238} U
LEU-COMP-THERM-017	1	1.0000	310	^{206,207,208} Pb, ^{235,238} U



Fig. 1. Flow chart diagram depicting the nuclear data uncertainty reduction process. Integral benchmarks are proposed as a second level of constraint in the TMC methodology. Feedback from updated parameter distributions after introducing integral experimental constraints can be given to model calculations for possible improvement.

Fig. 1. As can be seen from the figure, model calculations are compared with differential experimental data and uncertainty is assigned to each model parameter in the TALYS code (Koning et al., 2007). The model parameters are then varied all together within the model parameter uncertainties to create a large set of random nuclear data libraries (Koning and Rochman, 2012). In this way, differential experimental data serves as a first level of constraint for the model parameters used in the TALYS based code system within the Total Monte Carlo (TMC) methodology. The TMC method has been presented extensively in the following references (Koning and Rochman, 2008, 2012; Alhassan et al., 2015a; Rochman et al., 2009). As a second level of constraint, weights are assigned to the nuclear data libraries depending on their agreement with the benchmarks observable (e.g. flux, k_{eff}). The benchmark observable could vary depending on the type of benchmark. In this work, we have used benchmarks from the ICSBEP handbook and consequently only $k_{\rm eff}$ have been used as the benchmark observable. However the method could be applied to other types of benchmarks and consequently, other types of benchmark observables can be utilized. The weighted nuclear data libraries are used for a specific reactor system, referred here to as the application case, to reduce the nuclear data uncertainty in a reactor response parameter such as the $k_{\rm eff}$. In principle also, other reactor response parameters could have been investigated. However, due to computational resource constraints, only the $k_{\rm eff}$ was analyzed in this work. The temperature coefficients, for example, are computed by simulating reactor criticality (k_{eff}) between two perturbed configurations, these coefficients are dependent on the $k_{\rm eff}$ and therefore the uncertainty in these parameters will principally come from uncertainty in the $k_{\rm eff}$ as shown in Alhassan et al. (2015a).

4.1. Benchmark uncertainty

In Alhassan et al. (2014b), the acceptance interval (F_E) and weights (w_i) were computed taken into consideration only the evaluated benchmark uncertainty (σ_E) given in International Handbook of evaluated Criticality Safety Benchmark Experiments (2011). This uncertainty normally contains information on uncertainties in geometry, material compositions and experimental setup etc., nuclear data uncertainties were not taken into account. However, uncertainties from geometrical modeling of the benchmark in e.g. MCNPX, the calculation bias, the uncertainties from statistics (in the case of a Monte Carlo code) and the uncertainties in nuclear data of all isotopes contained in the benchmarks have impact on the calculation of the benchmark observable. To use a benchmark to reduce uncertainties therefore, we take all these uncertainties into account by computing a combined benchmark uncertainty for a particular benchmark (B) and isotope (j) given as:

$$\sigma_{B,j}^2 = \sigma_E^2 + \sigma_{C,j}^2 \tag{1}$$

where σ_c , the uncertainty in the calculation which takes into account the uncertainties in nuclear data of all isotopes within the benchmark other than the isotope whose uncertainty is being reduced, the uncertainties from geometrical modeling, the computational bias and the uncertainties from statistics, is expressed as:

$$\sigma_{C,j}^{2} = \sum_{\substack{\text{over all } p, \\ where \ p \neq i}} \sigma_{ND,p}^{2} + \sigma_{calc,bias}^{2} + \sigma_{geo,mod}^{2} + \sigma_{stat}^{2}$$
(2)

where *p* is the index for the different isotopes contained in the benchmark, $\sigma_{ND,p}$ is the nuclear data uncertainty of the benchmark for *p*th isotope and *j* is the isotope which we currently try to reduce its nuclear data uncertainty, $\sigma_{calc,bias}$ which is the computational bias, takes into account the uncertainty from the numerical methods used to solve the transport equation, $\sigma_{geo,mod}$ is geometrical modeling uncertainties, σ_{stat} is the statistical uncertainty in the case where a Monte Carlo code is used. In this work however, only $\sigma_{ND,p}$ was considered. Since enough computational time was invested to achieve small statistical uncertainties, the statistical uncertainty term was neglected. Similarly, because the integral experiments are clean and simple benchmarks, it was assumed in this work that the geometries of the benchmarks were modeled to a very high degree of accuracy and therefore the uncertainties due to geometrical modeling was neglected. Since the much validated Monte Carlo code (MCNPX) was used in this work, the computational bias term was assumed small and not included in this work.

If we consider reducing ²³⁹Pu nuclear data uncertainties using the pmf1c1 (PU-MET-FAST-001 case 1) benchmark which has the following isotopic composition: 95.2 at.% ²³⁹Pu, 4.5 at.% ²⁴⁰Pu, 0.3 at.% ²⁴¹Pu and 1.02 wt.% of gallium; neglecting cross correlation between isotopes, and neglecting also the calculation bias, statistical and geometrical modeling uncertainties, Eq. (1) becomes:

$$\sigma_{B,^{239}Pu}^2 = \sigma_E^2 + \sigma_{ND}^2(^{240}Pu) + \sigma_{ND}^2(^{241}Pu) + \sigma_{ND}^2(Ga)$$
(3)

where $\sigma_{B_{2}^{239}Pu}$ is the benchmark uncertainty when we want to use the benchmark to reduce the nuclear data uncertainty of ²³⁹Pu; $\sigma_{ND}(^{240}Pu)$, $\sigma_{ND}(^{241}Pu)$ and $\sigma_{ND}(Ga)$ are the nuclear data uncertainties of the other plutonium isotopes and gallium contained in the pmf1c1 benchmark respectively. In this work however, since the pmf1c1 benchmark is dominated by the uncertainties of the fissionable nuclides, $\sigma_{ND}(Ga)$ was not taken into account.

4.2. Correlation between application and benchmark

For a particular benchmark to be used for nuclear data uncertainty reduction for a specific application, a few criteria has to be fulfilled. The benchmark needs to be sensitive to the isotope under consideration, i.e., $\sigma_{i,ND}^2$ should be as high as possible, where j is the isotope under consideration. It should also have a combined benchmark uncertainty, $\sigma_{B,i}^2$ (see Eqs. (1) – (3)) as small as possible. Furthermore, the correlation (R), between the application case and the benchmark under consideration needs to be considered. More specifically the absolute value of the correlation should be as high as possible. The computation and interpretation of R is considered in this section. A study on how to select benchmarks for reactor calculations is presented in Alhassan et al. (2014b, 20156). In other studies, a representativity factor is used (Aliberti et al., 2006; Aliberti et al., August 2007), which makes use of sensitivity coefficient vectors and nuclear data covariance information to judge the applicability of critical experiments to actual reactor applications. This approach is however deterministic, based on the General Perturbation Theory (GPT) and also uses the multigroup energy structure. In this work however, an attempt is made to evaluate the applicability or the relevance of critical experiments for uncertainty reduction based on the Monte Carlo approach, starting from basic nuclear physics. The correlation coefficient computed between the $k_{\rm eff}$ values of the application case and the benchmark can be expressed as:

$$R = \frac{\sum_{i=1}^{n} \left(k_{\text{eff}(i)}^{\text{app}} - \overline{k_{\text{eff}}^{\text{app}}} \right) \left(k_{\text{eff}}^{B} - \overline{k_{\text{eff}}^{B}} \right)}{(n-1)\sigma_{k_{\text{eff}}^{\text{app}}}\sigma_{k_{\text{eff}}^{B}}}$$
(4)

where *n* is the number of random nuclear data files, k_{eff}^{app} and k_{eff}^{B} are the k_{eff} values for the i^{th} random file for the application case and the benchmark respectively, \overline{k}_{eff}^{app} and \overline{k}_{eff}^{B} are their mean values and $\sigma_{k_{eff}^{app}}$ and $\sigma_{k_{eff}^{B}}$ are their standard deviations.By using R in Eqs. (7) and (9) as presented in Sections 4.3 And 4.4 respectively, we ensure that a benchmark with for example, a 100% ²³⁹Pu composition, and having a high absolute value of R, will be a better candidate for the reduction of ²³⁹Pu nuclear data uncertainty of the application case compared to a benchmark with similar amounts of ²³⁹Pu with the application case but with a lower R. As a rule of the thumb, a limit of R > 0.3 is set for the correlation coefficient. This limit has however been chosen arbitrarily.

4.3. Binary accept/reject method

It was demonstrated earlier in Alhassan et al. (2014a) that, by setting a more stringent criteria for accepting random files based on integral benchmark information, nuclear data uncertainty could be reduced further. In Alhassan et al. (2014a) however, arbitrary χ^2 limits were set on accepting random files using criticality benchmarks without including evaluated benchmark uncertainty information. As an improvement to this method, benchmark uncertainty information was included to the uncertainty reduction process by computing an acceptance interval which was proportional to the benchmark uncertainty and presented in Alhassan et al., 2014b). The method made use of prior information included in the random nuclear data libraries produced using the TALYS based system, which implicitly included nuclear data covariance information from differential experiments. The nuclear data uncertainties in the observed prior were then further reduced by constraining the files using evaluated benchmark uncertainty information by calculating an acceptance band (F_E) , which constituted the 'a posteriori' uncertainties on the response parameters.

By introducing a proportionality constant equal to the inverse of the Pearson correlation coefficient computed between the application case and the benchmark, we were able to assign smaller acceptance intervals to strongly correlated benchmarks while weakly correlated benchmarks were assigned with larger intervals. In this work, a similar approach is presented but instead of constraining the random files with an acceptance band that only takes the evaluated benchmark uncertainty into consideration, we calculate F_E using instead, a combined benchmark uncertainty which is given in Eq. (1).

4.3.1. Acceptance interval (F_E)

To include benchmark uncertainty information, we propose an acceptance interval (F_E) which is directly proportional to the combined benchmark uncertainty ($\sigma_{B,j}$) for the j^{th} isotope, given in Eq. (1):

$$F_E \propto \sigma_{B,j}$$
 (5)

By introducing a proportionality constant κ given as the inverse of the Pearson correlation coefficient (*R*) computed between the benchmark and the application case, Eq. (5) becomes:

$$F_F = \kappa \sigma_{Bi} \tag{6}$$

where κ is expressed as:

$$\kappa = \frac{1}{|R|} \tag{7}$$

For the practical implementation of the binary accept/reject method, we consider the following: If *i* denotes the random files (random nuclear data) and $k_{eff(i)}$, a probability distribution function bounded by an acceptance band $[-F_E, +F_E]$. Let the maximum value of $k_{eff(i)}$ be denoted by $k_{eff}^{Max} = k_{eff,exp}^B + F_E$ and the minimum value, $k_{eff}^{Min} = k_{eff,exp}^B - F_E$, where $k_{eff,exp}^{Bax}$ is the evaluated experimental value of the benchmark observable. If an acceptance range is defined as $k_{eff}^{Min} \le k_{eff(i)} \le k_{eff}^{Max}$, any random file *i* that falls within this range is accepted as a realization of $k_{eff(i)}$ and therefore is assigned a binary value of one while those that do not meet this criteria take binary values of zero and are therefore rejected.

A posterior distribution of a parameter of interest (k_{eff} for example) can be obtained (using the accepted files) together with their mean and standard deviation which normally, should be narrower in spread than the prior distribution. In Fig. 2, a correlation plot example between the application case (ELECTRA) and the ²³⁹Pu Jezebel benchmark is presented showing the evaluated benchmark k_{eff} value and the corresponding acceptance band (F_E). By setting $\kappa = 1/|R|$, we assign smaller acceptance intervals (*F_E*) to strongly correlated benchmarks while weakly correlated benchmarks are assigned with larger acceptance intervals (F_E). In theory, κ could have been set to 1 for all benchmarks implying that all the benchmarks have the same weights. However, letting $\kappa > 1$, is a more conservative method and in practice, less weight is given to benchmarks with weak correlation to the application case i.e. we choose to accept a lot more random files for the weakly correlated benchmarks. Even though some of these random files might contain large errors for example in the thermal region, this effect will be relatively small in the fast region where the application case (ELECTRA) is used. For example, an R = 1 will give a $\kappa = 1$ implying that random files that fall within $1\sigma_B$ of the combined benchmark uncertainty are accepted, similarly a benchmark with a correlation coefficient of R=0.5, gives an acceptance interval of $2\sigma_B$.

There are however possible drawbacks to this methodology:



Fig. 2. k_{eff} correlation plot between ELECTRA and the ²³⁹Pu Jezebel benchmark showing the acceptance band (F_E). A correlation coefficient of R = 0.84 and an acceptance band $F_E = \pm 525$ pcm were obtained.

- For this method to be applicable, correlation coefficients between the application case and the benchmarks must be known and this involves a large number of reactor calculations and hence, computational time. This problem can however be solved by establishing a lookup validation database with information on random files performance on a wide range of different benchmark cases.
- 2) There is also the possibility of running into a situation where the number of random files that lie within F_E are so small that the uncertainty of the nuclear data uncertainty computed for the posterior distribution becomes very large. In such a situation, valuable feedback information is given to the prior for a further reduction of sampling widths used in sampling model parameters in the TALYS code.

4.4. Reducing uncertainty using the likelihood function

A more rigorous method is to base the uncertainty reduction on the likelihood function. Calibration of nuclear data using differential information has been performed by many authors (Smith, 2004; Duan et al., 2014; Helgesson et al., 2015). In Helgesson et al. (2015), file weights proportional to the likelihood function were assigned to the TENDL random files depending on how well they agreed with differential cross-section measurements:

$$w_i = \frac{e^{-\frac{1}{2}\chi_i^2}}{e^{-\frac{1}{2}\chi_{min}^2}}$$
(8)

where *i* is the random file number, w_i is the weight for the random file *i*. Experimental uncertainties and their correlations were included by computing a generalized χ_i^2 which takes into consideration the differential experimental covariance matrix and their correlations for the random file *i*.A similar approach is applied to nuclear data uncertainty reduction for reactor safety parameters, however, using a modified likelihood function computed by introducing integral benchmark experiment information and their correlations with an application case. Using TENDL random nuclear data libraries as our prior, file weights are assigned to each random file depending on their quality with respect to a benchmark value. Similar to the binary accept/reject case, the correlation between the benchmark and the application case is taken into account by introducing the Pearson correlation (*R*) as presented in Eq. (9):

$$w_{i,j} = \frac{e^{-\frac{1}{2}\chi_i^2 \left| R \right|}}{e^{-\frac{1}{2}\chi_{min}^2 \left| R \right|}}$$
(9)

where χ^2 is expressed by:

$$\chi_{i,j}^{2} = \frac{\left(k_{\text{eff}(i)}^{B} - k_{\text{eff},\text{exp}}^{B}\right)^{2}}{\sigma_{B,j}^{2}}$$
(10)

where, $\sigma_{B,j}^2$ which is the combined benchmark uncertainty for the benchmark *B* for the *j*th isotope whose nuclear data uncertainty is being reduced, is given in Eq. (1); $k_{\text{eff}(i)}^{B}$ is the calculated benchmark value for the *i*th random file and k_{eff}^{B} is the evaluated experimental value of the benchmark observable. Introducing the correlation coefficient (R) into Eq. (9) is a compromise between acquiring good accuracy and still preserve random files in the case where there is a weak correlation between the systems. After the computation of the weights, the weighted moments of the distributions can also be calculated. The advantage of this method is that no information is discarded and the full information from the benchmarks and the application case are used when evaluating the ND uncertainty distributions, since the tails are not cut as they are in the binary accept/reject method outlined in Section 4.3. The downside to this method is however that, given that model parameters are sampled from a wide probability distribution, a number of unlikely parameter combinations with very small weights will be produced. This will result in longer processing and reactor calculations time. To address this, Russian roulette can be used.

4.5. Simulations

For the variation of nuclear data, the classical one-at-a-time approach (Cacuci, 2010) was used. This approach was used since our goal is to identify the nuclear data inputs that have significant impact on the uncertainty of the output (the local effect) for uncertainty reduction purposes. To take into account the interactions between different input parameters (nuclear data by isotope), the random nuclear data libraries for all isotopes could have been varied simultaneously; this however, gives the global effect. Simultaneous variation has not been used in this work.

In this work, 300 random files of ²³⁹Pu, ²⁴⁰Pu, ²⁴¹Pu, ²⁰⁶Pb, ²⁰⁷Pb, ²⁰⁸Pb, ²³⁵U and ²³⁸U were each varied one after the other while all other isotopes were maintained as the reference library; JEFF-3.1 for ELECTRA and ENDF/B-VII.0 for the benchmarks. These libraries were used because they were the reference libraries that came with the versions of the SERPENT (Leppänen, 2013) and MCNPX (Briesmeister, 2000) codes used in this work.

For the application case (ELECTRA), criticality calculations were performed for a total of 500 k_{eff} cycles with 50,000 source neutrons corresponding to 25 million particle histories (with an average statistical uncertainty of 22 pcm) using the SERPENT code version 1.1.17 (Leppänen, 2013). For the benchmark cases, simulations were performed using the MCNPX code version 2.5 (Briesmeister, 2000) with 5000 neutron particles for 500 criticality cycles skipping the first 10 cycles resulting in an average statistical uncertainty of 47 pcm for the ²⁰⁸Pb case and 43 pcm for the ²⁴⁰Pu case. The seed of the MCNPX code was changed for each random run using the DBCN card. The calculation time for one random file calculation with, e.g., the ²³⁹Pu case, takes typically 1.65 min for the pmf2c1 benchmark case while it takes 293 CPU seconds for the application case (ELECTRA). It takes typically 13.89 min for the 208 Pb in the case of the hmf57c2 benchmark.

5. Results and discussion

5.1. Application case against benchmark correlations

In Fig. 3, examples of correlations between the application (ELECTRA) vs. benchmark (PU-MET-FAST) cases due to the variation of 239 Pu nuclear data are presented. Strong positive correlations are observed between ELECTRA and the benchmarks with the highest correlation coefficient (R = 0.93) recorded between ELECTRA and the pmf5c1 benchmark.

This could be attributed to the strong similarity in spectra exhibited by ELECTRA and the 'pmf' benchmarks. Furthermore, the high correlations recorded, give an indication that the fission/absorption ratio of the benchmarks is representative of the application case (ELECTRA). The correlation between ELECTRA and the other benchmarks are presented later in Section 5.2, Tables 4–6.

5.2. Nuclear data uncertainty reduction

For the computation of the combined benchmark uncertainty expressed in Eq. (1) for the reduction of 239 Pu and 240 Pu nuclear data uncertainty, only the uncertainties of the fissionable nuclides were considered in this work. This is because, it was observed that the nuclear data uncertainties of the pmf benchmarks were dominated by the uncertainties in the fissionable nuclides. Similarly, for the reduction of 208 Pb nuclear data uncertainties, only the uncertainty of lead nuclear data and that of the fissionable nuclides (235,238 U and 239,240 Pu in the case of pmf35c1) were considered since it was observed that the uncertainties of these nuclides dominate in the case of the lead sensitive benchmarks.

In Tables 2 and 3, the uncertainties of ^{239,240,241}Pu and, ^{208,207,206}Pb and ^{235,238}U nuclear data for a set of plutonium and

Table 2



Benchmark category	$\sigma_{ND}(^{239}\text{Pu})$	$\sigma_{ND}(^{240}\text{Pu})$	$\sigma_{ND}(^{241}\text{Pu})$
PU-MET-FAST-001	962 ± 42	178 ± 8	36 ± 3
PU-MET-FAST-002	826 ± 36	833 ± 34	254 ± 11
PU-MET-FAST-005	954 ± 42	192 ± 8	31 ± 4
PU-MET-FAST-008	939 ± 41	195 ± 8	28 ± 4
PU-MET-FAST-009	925 ± 41	186 ± 8	33 ± 3
PU-MET-FAST-010	906 ± 41	177 ± 8	30 ± 4
PU-MET-FAST-011	813 ± 36	191 ± 8	23 ± 5
PU-MET-FAST-012	948 ± 42	83 ± 6	36 ± 7
PU-MET-FAST-013	1004 ± 44	84 ± 4	7 ± 1
PU-MET-FAST-035	951 ± 42	68 ± 4	-
PU-MET-INTER-002	1267 ± 56	187 ± 8	22 ± 5

lead sensitive benchmarks are presented respectively. These uncertainties were computed using the TMC methodology and used in the computation of the combined benchmark uncertainty. From Table 2, it can be observed that the uncertainties of ²³⁹Pu nuclear data dominate in the case of the plutonium sensitive benchmarks except in the case of the pmf2c1 benchmark where relatively large ²⁴⁰Pu and ²⁴¹Pu nuclear data uncertainties were recorded. The large ²⁴⁰Pu and ²⁴¹Pu uncertainties obtained for the pmf2c1 benchmark is because of the relatively large amounts of ²⁴⁰Pu and ²⁴¹Pu contained in the pmf2c1 and its relatively high sensitivity to the variation of ²⁴⁰Pu and ²⁴¹Pu nuclear data. In the case of the lead sensitive benchmarks, as can be observed from Table 3, the uncertainties of ²⁰⁸Pb and ²³⁵U dominate. In Fig. 4, *k*_{eff} distributions due to the variation of ²³⁹Pu nuclear data after implementing the method of assigning file weights based on the likelihood function is presented using benchmarks for the ELECTRA reactor. It can be observed from the figure that, the posterior distributions. This can be



Fig. 3. Examples of correlation between the application (ELECTRA) and benchmark cases due to the variation of 239 Pu nuclear data. Top left: pmf1c1 vs. ELECTRA (R = 0.85), top right: pmf2c1 benchmark vs. ELECTRA (R = 0.83), bottom left: pmf5c1 vs. ELECTRA (R = 0.93) and bottom right: pmf8c1 vs. ELECTRA (R = 0.93). Note that 'c' does not imply cylindrical assembly as sometimes used (International Handbook of evaluated Criticality Safety Benchmark Experiments, 2011). In this paper, 'c' denotes the case of the benchmark. 300 random 239 Pu nuclear data were used.

Table 3

^{208,207,206}Pb and ^{235,238}U nuclear data uncertainties for a set of lead sensitive benchmarks computed using the TMC method. 300 random nuclear data files were used for all isotopes. PU-MET-FAST-035 benchmark is a plutonium sensitive benchmark and does not contain uranium - its uncertainties due to plutonium isotopes are given in Table 2.

Benchmark category	Case	$\sigma_{ND}(^{208}\text{Pb})$	$\sigma_{ND}(^{207}\text{Pb})$	$\sigma_{ND}(^{206}\text{Pb})$	$\sigma_{ND}(^{235}\text{U})$	$\sigma_{ND}(^{238}\text{U})$
PU-MET-FAST-035	1	430 ± 18	104 ± 5	89 ± 4	_	_
HEU-MET-FAST-027	1	450 ± 19	80 ± 4	75 ± 4	1130 ± 46	38 ± 3
HEU-MET-FAST-064	1	1124 ± 46	174 ± 8	171 ± 7	1045 ± 43	5 ± 1
HEU-MET-FAST-057	1	1002 ± 41	154 ± 7	163 ± 7	1071 ± 44	24 ± 4
HEU-MET-FAST-057	2	785 ± 32	129 ± 6	126 ± 6	1108 ± 45	27 ± 4
HEU-MET-FAST-057	3	1090 ± 45	169 ± 7	164 ± 7	1047 ± 43	19 ± 5
HEU-MET-FAST-057	4	737 ± 30	123 ± 6	119 ± 5	1102 ± 45	26 ± 4
HEU-MET-FAST-057	5	1168 ± 49	179 ± 8	181 ± 8	1043 ± 43	7 ± 1
LEU-COMP-THERM-010	21	410 ± 18	137 ± 7	66 ± 7	568 ± 25	105 ± 7
LEU-COMP-THERM-017	1	208 ± 10	76 ± 6	56 ± 6	376 ± 16	134 ± 7



Fig. 4. *k*_{eff} distributions due to the variation of ²³⁹Pu nuclear data after combining prior information with integral benchmark information from pmf1c1 (top left), pmf9c1 (top right), pmf10c1 (bottom left) and pmf11c1 (bottom right) benchmarks for the ELECTRA reactor using the method of assigning file weights based on the likelihood function. 'c' denotes the case of the benchmark.

attributed to the high sensitivity to the variation of ²³⁹Pu nuclear data of the pmf benchmarks and the strong correlation obtained between the pmf benchmarks and ELECTRA due to ²³⁹Pu nuclear data variation. Furthermore, the posterior distribution is greatly affected by the combined benchmark uncertainty; a small combined benchmark uncertainty could result in a much narrower posterior distribution and hence in a larger reduction in the posterior uncertainty. For the reduction of ²³⁹Pu nuclear data uncertainty, relatively smaller combined benchmark uncertainties were obtained.

In Tables 4 and 5, the ²³⁹Pu and ²⁴⁰Pu nuclear data uncertainty results obtained from the prior and posterior distributions using the binary accept/reject and the method of assigning file weights based on the likelihood function for the ELECTRA reactor are presented respectively. The PU-MET-FAST and PU-MET-INTER-035 benchmarks and, 300 ²³⁹Pu and ²⁴⁰Pu random nuclear data files were used. Very strong correlation coefficients are recorded for all benchmarks in the case of the variation of ²³⁹Pu nuclear data. This is because the benchmarks under consideration exhibit similar spectra with the application case (ELECTRA). Similarly, because of

the similarity in spectra, very strong correlations are recorded between ELECTRA and all benchmarks due to the variation of ²⁴⁰Pu random nuclear except in the case of the pmf12c1 benchmark where a moderately strong correlation coefficient was obtained.

Using the pmf (PU-MET-FAST) and pmi (PU-MET-INTER) benchmarks as presented in Table 4, the uncertainty due to ²³⁹Pu nuclear data for the application case (ELECTRA) was reduced from a high of 745 \pm 33 to the lowest value of 152 \pm 20 (representing a 80% reduction) for the binary accept/reject using the pmf12c1 benchmark, and from 745 \pm 33 to 178 \pm 22 (representing a 76% reduction) using the pmf13c1 benchmark the method of assigning file weights. The pmf13c1 ability to significantly impact the posterior uncertainty comes from its rather small combined benchmark uncertainty of 131 pcm and its high sensitivity to the variation of ²³⁹Pu nuclear data. Despite the fact that pmf8c1 has a much smaller evaluated benchmark uncertainty of 60 pcm and a higher correlation coefficient of 0.92 when compared with the pmf13c1 benchmark, a 65% uncertainty reduction was achieved. This could be attributed to the different combined benchmark uncertainties computed for the two benchmarks; 206 pcm was obtained for the

Table 4

Table showing ²³⁹Pu nuclear data uncertainty results from prior distributions compared with the posterior (binary accept/reject and the method of assigning file weights based on the likelihood function) for ELECTRA using a set of plutonium sensitive benchmarks. Results in brackets for the two methods represent the percentage reduction in nuclear data uncertainty achieved. The correlation coefficient between the application case (ELECTRA) and various benchmarks are also presented. The PU-MET-FAST benchmark cases and 300 ²³⁹Pu random nuclear data files were used. Only case one of each benchmark was used.

Benchmark category	Correlation	Prior [pcm]	Accept/reject [pcm]	File weights [pcm]
PU-MET-FAST-001	0.835	745 ± 33	417 ± 36 (44%)	432 ± 36 (42%)
PU-MET-FAST-002	0.850	745 ± 33	574 ± 29 (23%)	620 ± 32 (17%)
PU-MET-FAST-005	0.925	745 ± 33	298 ± 45 (60%)	330 ± 45 (56%)
PU-MET-FAST-008	0.923	745 ± 33	263 ± 30 (65%)	288 ± 29 (61%)
PU-MET-FAST-009	0.884	745 ± 33	359 ± 29 (52%)	413 ± 31 (45%)
PU-MET-FAST-010	0.918	745 ± 33	285 ± 27 (62%)	336 ± 29 (55%)
PU-MET-FAST-011	0.941	745 ± 33	362 ± 34 (51%)	378 ± 33 (49%)
PU-MET-FAST-012	0.838	745 ± 33	152 ± 20 (80%)	182 ± 21 (76%)
PU-MET-FAST-013	0.837	745 ± 33	153 ± 21 (79%)	178 ± 22 (76%)
PU-MET-FAST-035	0.876	745 ± 33	426 ± 29 (43%)	475 ± 31 (36%)
PU-MET-INTER-002	0.770	745 ± 33	580 ± 103 (22%)	549 ± 88 (26%)

Table 5

Table showing ²⁴⁰Pu nuclear data uncertainty results from the prior distributions compared with the posterior (binary accept/reject and the method of assigning file weights based on the likelihood function) for ELECTRA using a set of plutonium sensitive benchmarks. Results in brackets for the two methods represent the percentage reduction in nuclear data uncertainty achieved. The correlation coefficient between the application case (ELECTRA) and various benchmarks are also presented. The PU-MET-FAST benchmark cases and 300 ²⁴⁰Pu random nuclear data files were used. Case one of each benchmark was used.

Benchmark category	Correlation	Prior [pcm]	Accept/reject [pcm]	File weights [pcm]
PU-MET-FAST-001	0.944	1046 ± 43	1046 ± 43 (0%)	1034 ± 43 (1%)
PU-MET-FAST-002	0.973	1046 ± 43	718 ± 34 (31%)	833 ± 40 (20%)
PU-MET-FAST-008	0.960	1046 ± 43	1046 ± 43 (0%)	1030 ± 43 (2%)
PU-MET-FAST-009	0.952	1046 ± 43	1046 ± 43 (0%)	1032 ± 43 (1%)
PU-MET-FAST-010	0.962	1046 ± 43	1046 ± 43 (0%)	1032 ± 43 (1%)
PU-MET-FAST-011	0.951	1046 ± 43	1046 ± 43 (0%)	1029 ± 44 (2%)
PU-MET-FAST-012	0.660	1046 ± 43	1046 ± 43 (0%)	1042 ± 43 (0%)
PU-MET-FAST-013	0.875	1046 ± 43	1046 ± 43 (0%)	1042 ± 43 (0%)
PU-MET-FAST-035	0.876	1046 ± 43	1046 ± 43 (0%)	1043 ± 43 (0%)
PU-MET-INTER-002	0.877	1046 ± 43	1046 ± 43 (0%)	1041 ± 53 (0%)

pmf8c1 while 131 pcm was obtained for the pmf13c1 benchmark. It should however, be noted that, few files were accepted in the case of the pmf12c1 and the pmf13c1 benchmarks with the accept/ reject approach. From the table, it can be observed that the results from both methods compared favorably. In the case of uncertainty reduction of ELECTRA due to ²⁴⁰Pu nuclear data presented in Table 5, small or no reduction in nuclear data uncertainties were recorded for all benchmarks except in the case of the pmf2c1 benchmark where an uncertainty reduction of 31% and 20% were obtained with the binary accept/reject and the method of assigning file weights respectively. This is not surprising since the pmf2c1 benchmark and ELECTRA exhibit similar spectra and the pmf2c1 is also highly sensitive to the variation of ²⁴⁰Pu nuclear data.

In Table 6, results showing the ²⁰⁸Pb nuclear data uncertainty obtained from the prior and posterior distributions using the

binary/reject and the method of assigning file weights are presented for the ELECTRA reactor. The correlation coefficients computed between ELECTRA and each benchmark are also presented. Results in brackets (in column 5 and 6) show the percent reduction achieved by implementing the two methods. The PU-MET-FAST, HEU-MET-FAST and LEU-COMP-THERM benchmark cases and 300 random ²⁰⁸ Pb nuclear data files were used. The prior uncertainty of the application case due to ²⁰⁸Pb nuclear data computed is 897 ± 37. Uncertainty reductions ranging from a minimum of 6% (lct17c1) to a maximum of 82% (hmf57c5) were obtained with the accept/reject method while with the method of assigning file weights, uncertainty reductions obtained ranged from 0% (lct17c1) to 46% (hmf57c5). A high reduction in ²⁰⁸Pb nuclear data uncertainties of 72% was also recorded with the hmf57c3 with the accept/reject method while a reduction of 41% was

Table 6

Table showing ²⁰⁸Pb nuclear data uncertainty results from prior distributions compared to the posterior (binary accept/reject and the method of assigning file weights) for ELECTRA using a set of plutonium sensitive benchmarks. Results in brackets for the two methods represent the percentage reduction in nuclear data uncertainty achieved. The PU-MET-FAST, HEU-MET-FAST and LEU-COMP-THERM benchmark cases and 300 random ²⁰⁸Pb nuclear data files were used.

Benchmark category	Case	Correlation	Prior [pcm]	Accept/reject [pcm]	File weights [pcm]
PU-MET-FAST-035	1	0.983	897 ± 37	814 ± 34 (9%)	818 ± 35 (9%)
HEU-MET-FAST-027	1	0.992	897 ± 37	765 ± 32 (15%)	813 ± 35 (9%)
HEU-MET-FAST-064	1	0.996	897 ± 37	485 ± 24 (46%)	615 ± 30 (31%)
HEU-MET-FAST-057	1	0.995	897 ± 37	506 ± 27 (44%)	698 ± 35 (22%)
HEU-MET-FAST-057	2	0.995	897 ± 37	641 ± 28 (29%)	720 ± 32 (20%)
HEU-MET-FAST-057	3	0.996	897 ± 37	250 ± 30 (72%)	531 ± 43 (41%)
HEU-MET-FAST-057	4	0.995	897 ± 37	653 ± 34 (27%)	819 ± 40 (9%)
HEU-MET-FAST-057	5	0.996	897 ± 37	159 ± 32 (82%)	488 ± 52 (46%)
LEU-COMP-THERM-010	21	0.773	897 ± 37	762 ± 35 (16%)	818 ± 39 (9%)
LEU-COMP-THERM-017	1	0.753	897 ± 37	845 ± 104 (6%)	896 ± 47 (0%)

obtained with the method of assigning file weights. It should however, be noted that, with the accept/reject method, very few files were accepted in the case of the hmf57c3 and hmf57c5 benchmarks and therefore uncertainty reduction with these benchmarks should be interpreted with caution. Even though similar correlation coefficients were obtained for the hmf57 cases as can be seen from Table 6, the differences in uncertainty reduction obtained could be attributed to the different combined benchmark uncertainties computed for each benchmark and the sensitivity of the benchmarks to ²⁰⁸Pb nuclear data. The differences in reduction obtained with the accept/reject approach and the methods of assigning file weights based on the likelihood function for the hmf57 cases is due to the high $k_{\rm eff}$ values obtained which resulted in the acceptance of only the low $k_{\rm eff}$ values that lie within the acceptance band for the binary accept/reject approach. The high $k_{\rm eff}$ values observed for the benchmarks cases except in the case of hmf57c4, give an indication that the current lead cross section sets have some inaccuracies (International Handbook of evaluated Criticality Safety Benchmark Experiments, 2011). The high correlation coefficients obtained between the ELECTRA and the pmf35c1 and hmf benchmarks could be attributed to the similar fast spectra exhibited by both the application and benchmark cases.

Relatively small or no uncertainty reductions were observed for the lct benchmark cases as can be seen in Table 6. These benchmarks have thermal spectra while the application case (ELECTRA) has a fast spectrum. Also, the fissionable nuclides in the lct benchmarks are Low Enriched Uranium (LEU) while the fuel of ELECTRA is made of plutonium nuclides and ²⁴¹Am. Uncertainty reduction of ²⁰⁷Pb and ²⁰⁶Pb using benchmark information was not possible since the lead sensitive benchmarks under consideration contain small amounts of ²⁰⁷Pb and ²⁰⁶Pb. Furthermore, the nuclear data uncertainties of these benchmarks are dominated by the uncertainties in ²⁰⁸Pb and the fissionable nuclides as can be seen from Table 3, which resulted in rather large combined benchmark uncertainties. Since the accept/reject method cuts off the tails of the distribution, the method of assigning file weights can be considered as a more rigorous estimation of the posterior uncertainty since it takes all data into account. It should however be noted here that, there is generally a trade off between a gain in computational time and results accuracy.

6. Conclusion

A binary accept/reject and a method of assigning file weights based on the likelihood function for nuclear data uncertainty reduction using integral benchmarks have been presented and compared. Based on these methods, updated covariance matrices and model parameter distributions can be obtained for the adjustment of model parameter uncertainties in the TALYS based code system. It was observed from the study that, a significant reduction in nuclear data uncertainty was obtained for some isotopes for ELECTRA after incorporating integral benchmark information. In the case of ²³⁹Pu nuclear data, uncertainty reduction ranging from 22% to 80% were achieved with the accept/reject and between 17% and 76% with the method of assigning file weights. Small or no reduction in nuclear data uncertainties were however observed for ²⁴⁰Pu and ²⁴¹Pu isotopes. In the case of ²⁰⁸Pb nuclear data, the largest uncertainty reduction of 82% and 46% were achieved after implementing the binary accept/reject and the method of assigning file weights respectively. It should be noted however, that, with the accept/reject approach, few files were accepted in the case of some benchmarks. These feedbacks could be provided to nuclear reactions model calculations, for possible adjustment of model parameter uncertainties in the TALYS code.

With the current advances in computational power, it is

expected that, these methods could be implemented in the Total Monte Carlo methodology for nuclear data uncertainty reduction. Using and combining information from multiple benchmarks for data assimilation, taking into consideration benchmark correlations, is planned for future work.

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