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Sample Size Optimization for Propagation of Manufacturing Uncertainties in Criticality Calculation Using Random Sampling Method

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***Abstract* – Random sampling method is adopted in many fields of engineering and is currently been used to propagate uncertainties from nuclear data to behavior parameters of nuclear systems. It is also of great importance to know the effect of uncertainties inherent to physical components in order to calculate the total uncertainty associated with a model simulation. The propagated uncertainty is part of criticality safety calculations and guide vendors about accepted tolerance limits of the parts.**

In this work random sampling method for quantifying manufacturing uncertainties is accomplished by determining variance on neutron multiplication factor due to physical parameter uncertainties. Sample size and computational uncertainty were varied in order to investigate sample efficiency and convergence of the method. Random sampling efficiency was improved through the use of an algorithm for selecting distributions. Mean range and standard deviation range were compared with reference true values in order to verify the sampling. Transport code MCNPX was used to simulate a benchmark experiment and allow the mapping, from uncertain inputs to uncertain outputs. Replication-based approach with internal measure of accuracy was defined as convergence criterion to the method.

For a fixed computational time, in order to reduce the variance of the uncertainty propagated, it was found, the sample of size 186 is the best alternative among the tested cases. It serves as a reference sample size for future use in sampling based method. If this method is used to propagate uncertainties to k_{eff} in determining the upper limit of criticality for example, the value of result is lower than the value obtained by mean of the conservative method, allowing design optimization.

***Keywords* – Random sampling, Uncertainty propagation, Monte Carlo, Criticality calculation, Sample size optimization.**

I. Introduction

Physical uncertainty reported by manufacturer is one of the components that must be taken into account for criticality safety assessment. A simple method to account for these uncertainties is the sampling based method, that is been used in many international programs like [1] and [2], for quantification of uncertainties in nuclear systems. Sampling based method is a global method for parameter uncertainty propagation. It addresses even highly nonlinear behavior in the parameter space [3]. Properties of this method include conceptual simplicity, ease of implementation and generation of uncertainty analysis results without the use of intermediate models [4]. In neutronics field, the interest when adopting sampling based methods for uncertainty analysis is on the highest source of uncertainties, thatis nuclear data ([5]- [8]).

Using sampling-based method with MCNPX transport code to evaluate k_{eff} uncertainty for a storage array of 30B UF6 containers, (9) has shown that the k_{eff} uncertainty caused by uncertainties in non neutronic parameters, i.e. physical components, might be comparable to those due to neutronic parameters.

Five basic components that underlie the implementation of a sampling-based uncertainty analysis are (i) definition of distribution to characterize uncertainties, (ii) generation of a sample in consistency with the distributions, (iii) propagation of the sample through the analysis to produce a mapping from analysis input to analysis output, (iv) determination and presentation of analysis results.

If the physical uncertainty is already characterized, by manufacturer e.g., the next step is improve the sampling efficiency, that can be described as the number of simulation runs required to obtain a certain level of accuracy on the targeted outcomes. The lower the number of runs required, the higher the efficiency and as a consequence computational expense is minimized. Non-collapsing and space-filling sampling designs like LHS [10] are more efficient than basic random sampling [11]. A straight method was used here to improve efficiency of sampling without space-filling tools. A simple algorithm was used to check if sample distributions are in accordance with sampling requirements before perform the mapping between model input and model output.

To perform the propagation of the sample through the fissile material system, Monte Carlo neutron transport codes are widely employed because of their capability to represent physical reality more accurately than deterministic methods. Despite the huge computational effort necessary to run the sample size of inputs, a significant amount of time can be saved if a converged spatial distribution of fission source is used for all simulations [12].

Besides the use of efficient sampling designs, the stability of the analysis outcomes must be confirmed. The variance on the targeted outcome divided by the current number of runs can be used in a convergence criterion [13]. Nevertheless, when the number of runs is predetermined, the random-sampling-based error estimates via variance on the mean is not valid and a replication-based approach can be used [11].

For the problem under consideration, random sampling approach results were verified through comparison with a reference value. Further the method was used to quantify

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variance on neutron multiplication factor due to manufacturing uncertainties. Standard deviation of 5 pcm (per cent mile or $\times 10^{-5}$) in the propagated uncertainties for 10 n-samples replicates was adopted as convergence criterion to the method. Sample size and computational uncertainty balance was followed in order to increase efficiency and confirm convergence. Further, 1σ uncertainty quantified by random sampling method were compared with 1σ uncertainty estimated by a conservative methodology.

II. Methodology

A. Random sampling based method

The Total Monte Carlo method for nuclear data uncertainty propagation, presented in [14] and [8] was used as a reference methodology. In their work, uncertainty of nuclear model parameters are determined by theoretical considerations and comparison of nuclear model results with experimental data, i.e. characterization of uncertainties. Generation of sample in consistency with normal probability distributions is the second step. Then they use a nuclear model code to produce a complete nuclear data library containing all cross sections, angular distributions, particle emission spectra, photon production etc. which in turn is processed by NJOY [15] and used in a Monte Carlo transport code to calculate integral quantities e.g. reaction rates. The method necessarily demands an automated process. The set of about 5000 results contain systematical uncertainties propagated from basic nuclear physics model and experiments.

In the present work sampling based method was adopted to propagate uncertainties from physical components with tolerance intervals already characterized by manufactures.

The disciplined and quality assured working method (with emphasis on reproducibility) was achieved through functions of R statistical environment [16] embedded in programming routines, implemented in Python language [17] in order to automate the process of sampling, running cases, collecting and processing results. Random number generator of R environment [18] was used generate samples of size *n* with a predetermined distribution.

Uncertainty quantification via random sampling is relatively simple but computationally expensive, as many runs are needed to sample the parameter space in a representative way. Sampling strategies that require less runs are termed more efficient. Hence, to improve efficiency, an algorithm was created to perform five steps before adopting a sample.

- if the tolerance interval is not informed, sample distributionisde limited within the confidence interval of *MAX confidence* from the mean. The value of $\pm 3\sigma$ is used as default;
- sample distribution is checked (if is a normal distribution being sampled, p-value must be higher than 0.05 in normality test);
- sample distribution must present skewness smaller than a predetermined threshold *MAX skewness*;
- relative deviation between sampled mean and requested mean must be less than a predetermined threshold *MAX mean*;
- relative deviation between sampled standard deviation and requested standard deviation must be less than a predetermined threshold *MAXsd*.

Therefore, the trial and error algorithm has the task of eliminating distributions that do not match the requirements specified for the random number generator with an certain accuracy level, for a fixed sample size *n*. It retains the first distribution that passes the test. Although it is not a rigorous approach, as will be seen in next section, the algorithm is sufficient to ensure efficient sampling without use of space-filling sampling designs.

When many uncertain parameters are set for an input (e.g. uncertainty quantification of *m* physical parameters), this sampling strategy is done for each parameter separately (e.g. *m* times). The results are *m* unordered lists of *n* components. The first value in each list will compose the first input. The second value will compose the second input and so forth until *n* inputs with *m* uncertain components are constructed and queued to run.

Monte Carlo transport code MCNPX [19] using ENDF/B-VII nuclear data evaluation was used to permit the propagation of the sample through the fissile material system and produce a mapping from analysis input to analysis output. The input files for this method are samples of size *n* MCNPX geometry input files. The uncertain variable sampled for verification was burnable poison radius described in Table 1. At the end of *n* calculations, *n* different k_{eff} values with their statistical uncertainties are obtained. For this probability distribution of k_{eff}, the standard deviation σ_{total} can be decomposed, to reflect two different effects [12]:

$$\sigma_{total}^2 = \bar{\sigma}_{comp.}^2 + \sigma_{input}^2$$
$$\bar{\sigma}_{comp.}^2 = \frac{1}{n}\sum_{i=1}^{n} \bar{\sigma}_{comp.,i}^2 \qquad (1)$$

MCNPX simulations provide an estimation of $\sigma_{comp.}$ (computational uncertainty), which can be used in (1) to extract σ_{input} (systematic uncertainty) by the square root of the sum of squares. A converged spatial distribution of fission source (SRCTP file) was used for all simulations in order to reduce the running time.

The replication-based approach described in [11] was adopted and internal measure of accuracy was used as convergence criterion to the method. The standard deviation for 10 n-samples replicates (σ_{input}^2 and $\bar{k}_{eff} = k_{eff}$ mean) must be within 5 pcm to pass the criterion. The 10 replicates are denoted distribution ID 1 to 10; ID 11 to 20; and so on. A MCNPX calculation of the benchmark experiment presented in section 2.2 with no uncertain parameters (i.e. not sampled, using only the Monte Carlo nuclear code) and computational uncertain set to 10 pcm is the reference solution to validate the method through comparison and agreement of k_{eff} probability distributions obtained by the replicates.

B. Source of uncertainties

Manufacturing uncertainties are the tolerance intervals assigned to parts or physical components for manufacturing purposes. To test the random sampling method it is necessary to select a transport code and some uncertain parameter.

The uncertain parameter used is a manufacturing tolerance described in the benchmark experiment document [20] and reproduced in Table 1. Burnable poison radius was selected as a reference true value of statistical quantities due to its significant influence in the system k_{eff} and its independence of others physical parameters, avoiding consider co-variances in the representation of uncertainties when applying the sampling based method.

Table1: Manufacturing uncertainty of burnable poison radius and its effect in k_{eff}.

Value	0.02425 cm
Uncertainty*	0.00025 cm
Number of measurements	90
Resolution**	0.0001 cm
Effect on k_{eff}	91 pcm
Distribution	Normal

**Standard deviation of the sample*
***Of measuring device*

The test problem under consideration is the MCNPX model of the open pool Material Test Reactor RA-6 (Argentina Reactor, Number 6), located in Centro Atomico Bariloche. Light water is used as coolant, moderator and reflector in the reactor core. Fuel elements are rectangular type, aluminum clad and fuel meat composed by 19.7% enriched uranium silicide USi_2 mixed with aluminum. Figure 1 presents details of RA-6 fuel element. Burnable poison are the cadmium wires in red color.

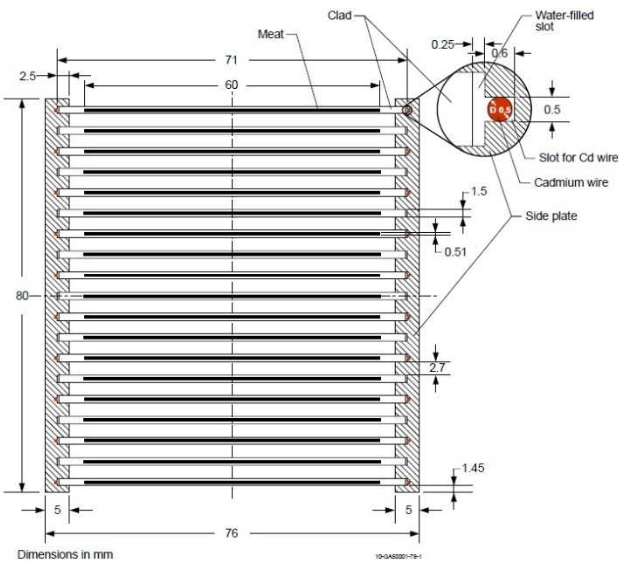


Fig.1.Geometric details of RA-6 Fuel Element, source: [20].

The notation "1σ" is used to represent one standard deviation from the mean. A normal probability distribution was assumed because the uncertainty is based in measurements and no skew information or the original values measured are available.

In the original document, a conservative method was used to determine deviation on k_{eff}, i.e. Δk_{eff}, running the model for the worst cases of the tolerance interval $[-1\sigma, +1\sigma]$, i.e. $\pm\Delta x$.

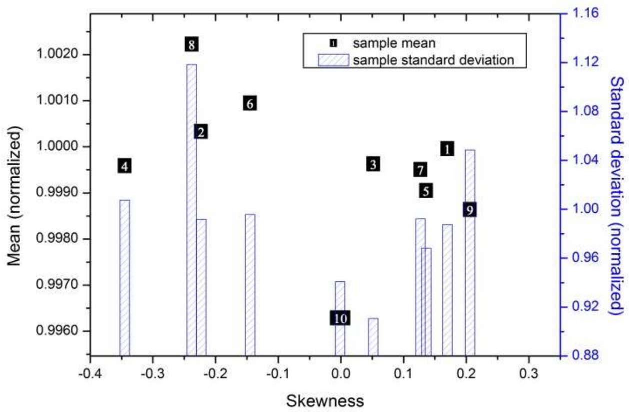
$$\Delta k_{eff} = \frac{\left|k_{eff}^{+\Delta x} + k_{eff}^{0}\right| + \left|k_{eff}^{-\Delta x} - k_{eff}^{0}\right|}{2} \quad (2)$$

Where k_{eff}^{0} is the neutron multiplication factor of the non pertur bed model. Table 1 presents 1σ uncertainty associated with the burnable poison radius and its effect on k_{eff} calculated using (2).

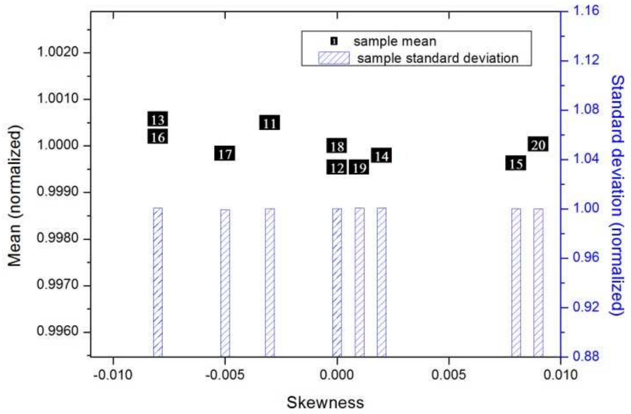
III. Results

A. Selecting relevant distributions - sampling verification

As mentioned in section 2.1 the method converges if the standard deviation on the input standard deviations for 10 n-samples replicates, i.e. the internal standard deviation, are within 5 pcm.Ten replicates of size 93, denoted ID 1 to 10, were generated from burnable poison radius and its associated uncertainty. Fig. 2a presents the relative mean, relative standard deviation and skewness of each replicate generated, with respect to the valuesrequired for sampling. In other words, random sampling was used, by means of the random number generator, without apply the algorithm described in section 2.1. Coordinate axes were normalized by reference true values of 0.02425 cm (burnable poison radius mean) and 0.00025 cm (1σ uncertainty) respectively. It is observed that the relative mean for 10 replicates ranges from approximately -0.4% to +0.2%, relative standard deviation ranges from -8% to +14% and skewness varies from approximately -0.35 to +0.2. Replicates ID 11 to 20 were generated using the trial and error algorithm implemented for this work. Obtainment of a n = 93 sample that meets the requirements-0.1% <MAXmean <0.1%; -0.01% <MAXsd<0.01%; -0.01 <MAXskewness <0.01 demanded around 5 minutes of running in a 3.3 GHz PC. Improvement in sampling efficiency can be seen in Fig.2b.



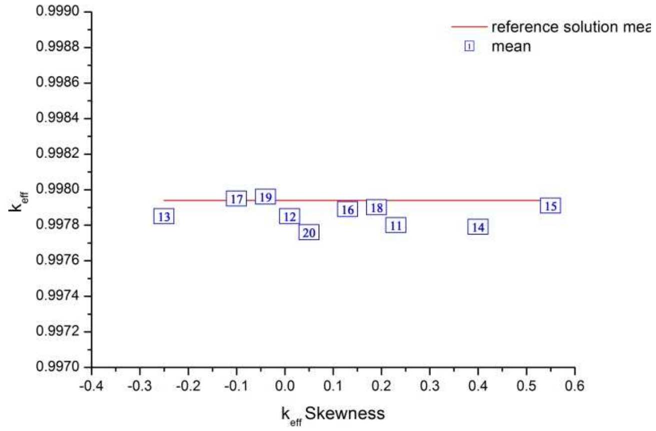
(a) Replicates ID1 to 10.



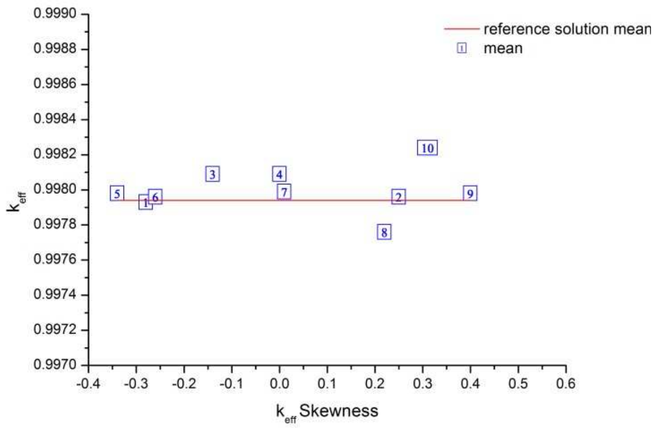
(b) Replicates ID11 to 20.

Fig.2. Mean and standard deviation as function of skewness on sample distribution normalized by reference quantities.

Figure 3a. and 3b. show fluctuations on mean and skewness on k_{eff} distribution for replicates ID 1 to 10 and ID 11 to 20, respectively.



(a) Replicates ID1 to 10.

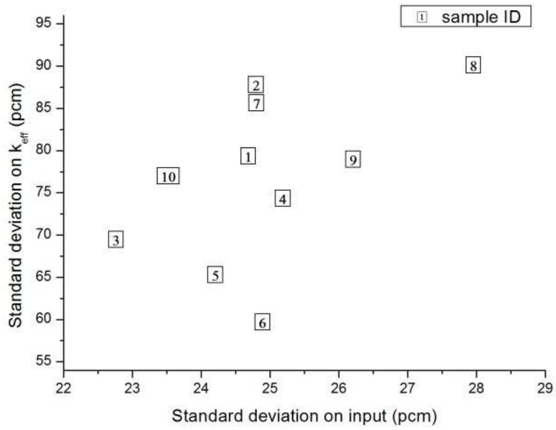


(b) Replicates ID11 to 20.

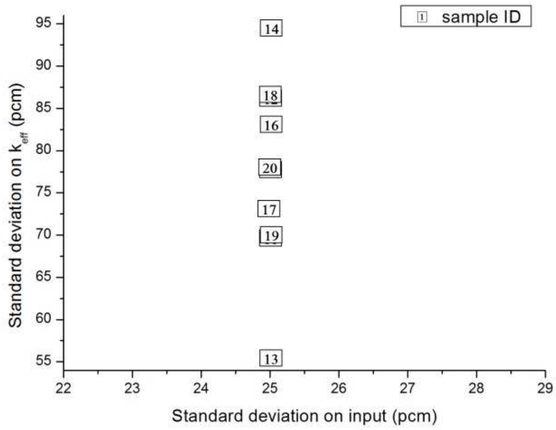
Fig.3. Mean and skewness of k_{eff} probabilitydistributions and benchmark experiment k_{eff} mean (reference solution).

Comparing the 2 sets of 10 replicates, internal standard deviation on k_{eff}mean is reduced by 44% (from 12.3 pcm to 6.8 pcm) reflecting the improvement on sampling efficiency of replicates ID 11 to 20. The reduction on skewness of k_{eff} probability distribution is insignificant.

Uncertainty propagated to k_{eff} as function of uncertainty in burnable poison radius is presented in Fig. 4. For a standard deviation nearly constant on input distribution (lower than 0.1% after use of the algorithm to select distributions), internal standard deviation on k_{eff} distribution of 10 replicates increases from 9.8 to 11.1 pcm. Despite the efficient sampling to represent input distribution with sample of size 93 and $\sigma_{comp} \approx 60$ pcm, reduction on variance of output distribution mean was not small enough to meet convergence requirement. Computational uncertainty ($\sigma^2_{comp.}$) and sample size are varied in next section in order to investigate the best approach to reach convergence for this study.



(a) Replicates ID1 to 10



(b) Replicates ID11 to 20.

Fig.4. Uncertainty in burnable poison radius (standard deviation) as function of propagated uncertainty (standard deviation on k_{eff}).

B. Optimization of sample size and computational uncertainty

Three sets of 10 replicates which demand the same computational time to run were used to determine the best balance between sample size and computational uncertainty configuration. The first set of cases, ID 11 to 20, had twice the number of histories run in MCNPX than the second set, with $\sigma_{comp.}$having a value of approximately 28.5 pcm. The second set of cases, ID 31 to 40, was configured with twice the sample size than the first set, i.e.

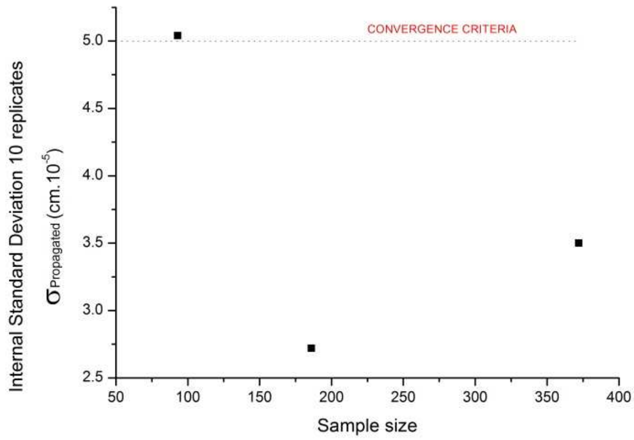
n = 186. The third set of samples, ID 41 to 50, has three times the number of samples of the first set and one third the histories run in MCNPX.

Table 2 gathers data of propagated uncertainty from the 3 sets of 10 n-samples as function of computational uncertaintyand sample size. Internal deviation is defined as the standard deviation (SD) on the input standard deviations (given in the fourth column) and the standard deviation (SD) on the k_{eff} mean (given in sixth column) of Table 2. For each set of 10 replicates, dispersion of k_{eff} standard deviation is illustrated in Fig. 5a and dispersion of k_{eff} mean (k_{eff}) is illustrated in Fig. 5b.

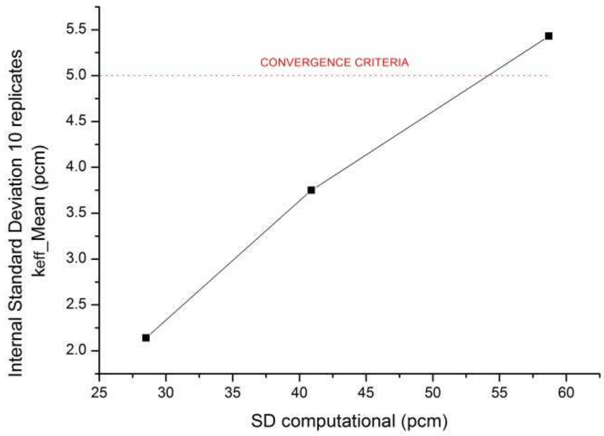
Table 2: Dispersion in 3 sets of 10 n-samples replicates that demand the same computational time to run.

ID	n	$\sigma^*_{comp.}$	σ^*_{input}	$\sigma^*_{internal}$ σ_{input}	k^*_{eff}	$\sigma^*_{internal}$ $\bar{k}_{eff}$
11	93	28.5	72.1	-	0.99787	-
12	93	28.4	72.4	-	0.99787	-
13	93	28.6	64.6	-	0.99786	-
14	93	28.5	74.4	-	0.99787	-
15	93	28.5	80.6	-	0.99788	-
16	93	28.5	75.9	-	0.99787	-
17	93	28.5	76.9	-	0.99784	-
18	93	28.4	75.4	-	0.99787	-
19	93	28.4	83.2	-	0.99792	-
20	93	28.4	76.6	-	0.99790	-
31	186	40.8	80.9	-	0.99789	-
32	186	41.2	76.0	-	0.99793	-
33	186	41.0	71.6	-	0.99788	-
34	186	40.9	72.7	-	0.99793	-
35	186	40.8	78.2	-	0.99792	-
36	186	40.7	76.2	-	0.99798	-
37	186	40.9	75.3	-	0.99791	-
38	186	40.8	76.1	-	0.99794	-
39	186	40.8	74.3	-	0.99790	-
40	186	40.8	78.1	-	0.99785	-
41	372	58.8	77.1	-	0.99795	-
42	372	58.4	77.6	-	0.99779	-
43	372	58.7	80.7	-	0.99792	-
44	372	58.9	75.8	-	0.99790	-
45	372	58.6	72.7	-	0.99785	-
46	372	58.9	74.4	-	0.99781	-
47	372	58.5	85.4	-	0.99787	-
48	372	58.7	76.4	-	0.99782	-
49	372	58.6	77.3	-	0.99784	-
50	372	58.9	76.6	-	0.99792	-
11-20	93	28.5[a]	75.2[a]	5.04**	0.99787[a]	2.14
31-40	186	40.9[a]	75.9[a]	2.72	0.99791[a]	3.75
41-50	372	58.7[a]	77.4[a]	3.50	0.99787[a]	5.43**

[a] *arithmetic mean of 10 n-run-set.*
* *Values expressed in per cent mile (pcm) or* $\times 10^{-5}$.
** *Fails the convergence criteria.*



(a)Effect on propagated uncertainty (dispersion of k_{eff} standard deviation for 10 replicates).



(b)Effect on k_{eff} (dispersion of k_{eff} mean for 10 replicates).

Fig.5. Balance between sample size and computational uncertainty.

Set ID 41 to 50 resulted a small internal deviation in input (propagated) but the internal deviation in $\bar{k}_{eff}$ is higher than 5 pcm. The comparison between set ID 11-20 results from section 3.1 and results from section 3.2 shows the reduction on internal deviation of input from 11.1 to 5.04 pcm after computational uncertainty is reduced. However the convergence criteria is still not reached.

Set of sample size 186 (ID 31 to 40) showed the smallest internal deviation (2.7 pcm) and was the only that meet the requirements for convergence. Therefore for a given fixed computational time, it is preferable to use n = 186 for sampling rather than to invest in reducing the computational uncertainty or double the sample size.

C. Comparison with conservative method

A direct comparison between sampling-based and conservative method to estimate variance on k_{eff} is presented in Table 3. As expected, the value of the effect on k_{eff} calculated by the sampling based method was lower than the value calculated by the conservative method. The 1σ uncertainty on k_{eff} calculated by the conservative method is estimated by the difference between cases in

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which the uncertain parameter takes the minimum and the maximum value of confidence interval of input parameter distribution (i.e. $\pm\Delta x$ on (3)). However uncertainty propagated by the sampling based method represents1$\sigma$of the distribution of k_{eff} . Uncertainty propagated by the sampling method was 84% of the uncertainty calculated by the conservative method. Taking into account that sampling basedmethods allow propagate many uncertainties in the same input, using the methodology described in section 2.1, the ratio can be even more realistic for a case when many manufacturer uncertainties are involved.

Table 3: Effect of propagation of burnable poison radius 1σ uncertainty on k_{eff} according to the method employed.

Conservative	Sampling-based	ratio
91.2 pcm	76.6	84%

IV. Conclusions

Samples had their statistical quantities followed and it wasverified the inefficiency of the random sampling to represent a requested distribution for the sample of size 93. In order to improve efficiency a trial and error algorithm was implemented to select sample distributions that match the quantities required. Statistical analysis carried out for individual replicated samples showed reduction in mean range, standard deviation range and skewness of 67%, 100% and 96% respectively (i.e. from [-0.4%,+0.2%], [-8%,+14%] and [-0.35,+0.2] to [-0.1%,+0.1%], [-0,01%,+0.01%] and [-0.01,+0.01]). Before map input uncertainty to output uncertainty, this result was verified through the comparison of the sample mean and standard deviation with mean and standard deviation reference true values (Fig. 2).

Uncertainty of burnable poison radius was propagated through sampling based method. In particular, k_{eff} uncertainty was quantified for the RA-6 Material Test Reactor using MCNPXinput parameters random sampling. Convergence criterion of internal standard deviation lower than 5 pcm (mean and standard deviation) for 10 n-size replicates was followed for three different configurations of sample size x computational uncertainty.

The case with sample size 186 (i.e. n = 186, $\sigma_{comp.} \approx 41$ pcm) resulted a lower variance in the uncertainty propagated and was the only passed the convergence criterion (10-replicates internal standard deviation of $\sigma_{input} \leq 5$ pcm and 10-replicates internal standard deviation of $\bar{k}_{eff}$ $\leq$5 pcm). This was the best alternative to quantify 75 pcm uncertainty (1σ) in reactor k_{eff} due to burnable poison radius uncertainty (Tab.2).

The comparison between sampling based method with a conservative method showed the uncertainty of burnable poison diameter propagated by the sampling method was 84% of the value calculated by the conservative method, indicating a potential space or materials optimization achieved by the use of a more realistic uncertainty quantification method in criticality safety analysis.

V. Acknowledgments

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