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Uncertainty Analysis of TREAT Standard Fuel Assembly and Minimum Critical Core Models

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Abstract - *This paper presents the uncertainty analysis of the original Minimum Critical Core of the TREAT reactor. A stochastic uncertainty analysis was performed on the contribution of geometric and composition specification of the assembly using Monte Carlo Neutronics methods. Results show that Boron contamination, Zr can thickness, Al can thickness and flat-to-flat distance of fuel blocks are the most significant design factors contributing to the variance.*

I. INTRODUCTION

The objective of the work reported in this paper is to quantify the uncertainties in the prediction of k_{eff} of a single assembly and the minimum critical core loading of the TREAT reactor which are attributable to uncertainties in the fuel material composition and geometry parameters. The work was based on stochastic sampling method and all neutronics calculations were performed using the Monte Carlo code SERPENT. The TREAT reactor is an air-cooled, graphite moderated, thermal test facility designed to evaluate reactor fuel and structural materials under severe reactor-accident conditions. [1] The minimum critical core configuration being studied in this paper was the steady-state core configuration when the reactor began operation in 1959.

Two major challenges were addressed in this work. First, the detailed boron contamination and its distribution in TREAT fuel assemblies were not available because of incomplete records. This led to difficulties in generating a boron sample distribution and required the development of a chi square weighting method which provided reasonable results. Second, uncertainties in the core calculation introduced by uncertainties in geometry parameters and their correlations were analyzed. The results provided important information for the continuing analysis in support of the TREAT reactor restart efforts.

II. THEORY

1. Description of the SERPENT Model

Figure 1 shows the minimum critical core configuration of TREAT. It consists 133 standard fuel assemblies, 8 control rod fuel assemblies and 16 Zircaloy-clad dummy fuel assemblies. Detailed description of the geometry of the configuration is given in [1]. The SERPENT model of TREAT standard fuel assembly is shown in Figure 2. The left most part in Figure 2 is the side view of the assembly, followed by the partial enlarged views of the fuel can outgas tube and the spacer. The right most part provides cross views of different sections of the fuel assembly. The control rod fuel assembly is a standard fuel assembly with a hole down to center to allow for vertical movements of control rods. The Zircaloy-clad dummy fuel assembly follows a similar design to the standard fuel assembly. There are two notable differences. First, the graphite-fuel blocks are replaced with graphite blocks. Second, the outgas tubes are removed since there is no fuel in the dummy assemblies.

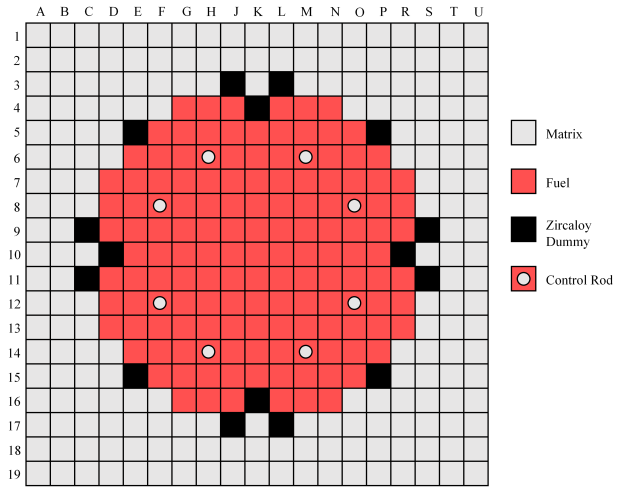

Fig. 1. TREAT minimum critical core configuration.

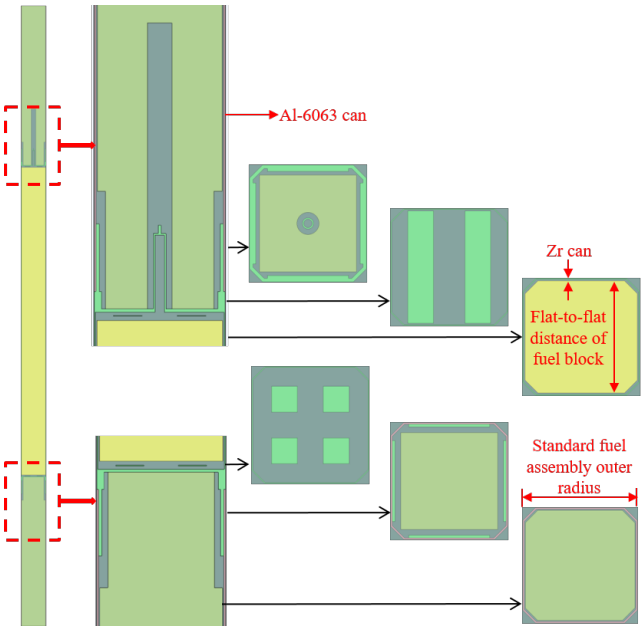

Fig. 2. TREAT standard fuel assembly SERPENT model.

An example uncertainty evaluation for infinite lattice fuel assembly model was given in [1]. Results from this analysis pointed out that uncertainties in the following five groups of factors are the most significant "contributors" of the uncertainties in the eigenvalue calculation. The sample space and distribution information for these parameters should be modeled as close to the operational history of TREAT as possible.

- Uranium vector: the weight percent of each uranium isotope (U234, U235, U236 and U238) among total uranium content in graphite fuel.
- Fuel composition: the weight % of each element in the graphite fuel (B, O, U, C, V, Fe).
- Al-6063 can related parameters: alloy composition, density, can thickness.
- Fuel block geometry: flat to flat distance of fuel block.
- Zr can related parameters: alloy composition, density, can thickness.

In the reference uncertainty analysis ([1]), the distributions of the material composition factors are assumed as normal distributions. The geometry factors such as Al-6063 can thickness and Zr can thickness are treated as uniformly distributed random variables. Besides these assumptions, some other distributions may describe the factors better. The following paragraphs provide possible tools and records from other references to re-estimate the distribution that each parameter follows.

2. Distribution of Boron Impurity

Boron content in the graphite fuel is one of the most significant uncertain factors observed. This uncertainty resulted directly from the procedure used to bake the fuel during the fuel fabrication of TREAT. Ref [2] noted that during the TREAT fuel baking procedure, boron loaded stainless steel was used as separator material between the assemblies to alleviate concerns with criticality which allowed boron to diffuse into core graphite. [3] To evaluate the boron contamination resulting from this fabrication procedure, 50 core graphite samples (a total of 1.25g) were tested. The samples were then separated into four groups and each group contained a different number of samples. Only the mean and average deviation values of each group were recorded. [4]

Two methods were evaluated to combine statistics from the four groups. The first method is inverse variance weighting in which the sample means $y_1,\ y_2, \ldots,\ y_k$ from k individual studies, with respective known variances $\sigma_1^2, \ldots,\ \sigma_k^2$ are evaluated using an inverse weighting procedure in which the variance of the weighted mean is minimized by $w_i = \frac{1}{\sigma_i^2},\ i = 1, 2, \ldots, k$. [5] In this case, the weighting factors are defined as:

$$w_i = (\frac{1}{\sigma_i^2})/(\sum_{j=1}^{k} \frac{1}{\sigma_j^2}),\ i = 1, 2, \ldots, k. \tag{1}$$

And the variance of the weighted mean $\sum_{i=1}^{k} w_i y_i$ is then defined as

$$\sum_{i=1}^{k} w_i^2 Var(y_i) = \frac{1}{\sum_{j=1}^{k} \frac{1}{\sigma_j^2}}. \tag{2}$$

Based on Eq. (1) and (2), the weighted mean ($\bar{y}$) and the standard deviation of this estimation ($\sigma_{\bar{y}}$) can be calculated and the boron content is therefore assumed to follow a normal distribution $\mathcal{N}(\mu = \bar{y}, \sigma = \sigma_{\bar{y}})$.

The second method was developed specifically for this work and is based on "chi-square weighting". It is based on the assumption that the boron impurity in core graphite follows a normal distribution. (Notice that it is assumed that there is no spatial dependency of boron contamination.) Under this assumption, the ratio between variances observed from the four groups and the actual distribution coefficient σ^2 follows chi-square distribution: [6]

$$(n_i - 1)\left(\frac{S_i^2}{\sigma^2}\right) \sim \chi^2(n_i - 1) \tag{3}$$

where n_i is the sample size of the i^{th} group and S_i^2 is the variance observed in the i^{th} group. $\chi^2(n_i - 1)$ denotes a chi-square distribution with the degree of freedom $(n_i - 1)$. Denote $v_i = \frac{S_i^2}{\sigma^2}$ and perform a variable transformation, the probability distribution function of v_i is obtained as

$$f(v_i) = (n_i - 1)\chi_{n_i - 1}^2 \tag{4}$$

Based on Eq. (4), the probability of having v_i in the range of $[0.9, 1.1]$ can be estimated. These probabilities were used as the weight of each group data to calculate weighted mean and variance results. Again the weighted mean and variance are used as the $\mu,\ \sigma^2$ coefficients for the normal distribution of boron.

Among the two methods, the first uses the standard deviation of the estimated distribution mean as the distribution coefficient. This significantly underestimates the real deviation among the Boron contamination distribution. The inverse variance weighting factors make the data group with the smallest variance become the most important part of the estimation. This may lead to inaccurate estimation. The second method estimates the distribution coefficients based on the same assumption used by the first method but with a more solid theoretical foundation. The k_{eff} calculated using the chi-square weighted boron contamination was closer to critical compared to result calculated with inverse variance weighted boron value.

3. Distribution of Geometry parameters

A uniform distribution was assumed for geometry factors in [1]. However, a triangular distribution may be more suitable in this case. [7] Characterised by three numbers $a,\ b$ and c, a triangular distribution is defined on the range $x \in [a, b]$ with probability density function

$$p(x) = \begin{cases} \frac{2(x-a)}{(b-1)(c-a)}, & a \le x \le c. \\ \frac{2(b-x)}{(b-a)(b-c)}, & c < x \le b. \end{cases} \tag{5}$$

While uniform distribution says that the value of the geometry factor may fall on any value within the range with same probability, triangular distribution defines a most "preferred" value and the upper/lower bounds for the factor. Triangular distribution can be asymmetric with respect to the expected value of the distribution. This makes it attractive when modeling TREAT as some of the factors were measured to follow an asymmetric distribution. An example is the density of graphite fuel.

4. Sample Generation

Table I summarizes the distribution information of the factors studied in the work. Notice that for Al-6063 can thickness and Zr-3 can thickness, uniform distribution was used in the standard fuel assembly model. This was based on Table 4.2 in Ref [1]. Then the distribution assumptions of these two factors were modified to triangular distributions in the minimum critical core model.

The sample generation procedures contain the following steps.

- Step 1: generate a data matrix $X \in \mathbb{R}^{n\times p}$ which represents n observations of p random variables. The variables follow multivariate joint normal distribution with an identity covariance matrix. This data matrix is called the "raw" sample here after. It is used as a "sample base" to generate samples for all the factors through probability distribution transformation. The reason for choosing multivariate joint normal distribution as the sample base is that only for this distribution, a diagonal covariance matrix implies independence. This is used as an important criteria in the later steps. Notice that to avoid ill-conditioned covariance matrix, n should be chosen much larger than p.

- Step 2: take $Y = XT$, T is a matrix operator. Detailed expression of T is given in the next subsection. This step is performed to eliminate the "artificial" covariance between random variables. Although the samples of different factors are generated independently, a non-diagonal covariance matrix is often observed in reality due to statistical fluctuations. For variables which follow joint normal distribution, this gives an "artificial" dependency. The effect brought by this may be weak or significant depends on the complexity of the model of interest. For the work presented in this paper, this step is designed to eliminate effects from outside the model as much as possible.

  After the first two steps, the random variable data matrix Y obtained should have a covariance matrix which is almost diagonal.

- Step 3: transfer each column of random variables back to the desired marginal distribution.

- Step 4: for those factors which are physically correlated, (for example, weight percentages of different elements in an alloy should add up to one, geometry parameters of different sections of assembly should align, etc.) keep one of the factors as a balance. For example, four random variables x_1, x_2, x_3, x_4 which represent the weight percentages of $U234$, $U235$, $U236$, $U238$. x_4 could be sampled as $100 - x_1 - x_2 - x_3$.

The steps established are to make sure that the "raw" samples generated are as independent as possible before transforming each variable back to its user defined marginal distribution. The raw samples were generated using multivariate joint-normal distribution. The operator T was applied to push the covariance matrix of the raw samples generated to "almost" diagonal. Joint-normal distributed variables with diagonal covariance matrix are guaranteed to be independent from each other. [8] Then, these independent random variables are transferred back to their marginal distributions and the physical correlations are built upon that. Unfortunately, geometry parameters are not like nuclear cross sections which have predefined covariance information. Hence the correlation between parameters has to be considered at the end.

For geometry parameters, when perturbation is added on one factor, sections adjacent to the section defined by the perturbed factor may be effected. The principle used for the work in this paper was to conserve the volume of unperturbed sections. In cases where volume conservation is not achievable, the effect will be pushed toward air filled sections. For example, when perturbing the Al-6063 can thickness, the outer radius of Al can was changed to reflect the perturbation while the inner radius was kept unchanged.

A. Determination of the T Operator

Taking N samples of the random variable x_i and x_j. the unbiased covariance of these two variables from this N set of samples is estimated as

$$cov(x_i, x_j) = \frac{1}{N-1}\sum_{k=1}^{N}(x_i^{(k)} - \mu_i)(x_j^{(k)} - \mu_j) \tag{6}$$

$$= \frac{1}{N-1}\sum_{k=1}^{N} x_i^{(k)} x_j^{(k)} - \frac{N}{N-1}\mu_i\mu_j \tag{7}$$

Given the data matrix $X \in \mathbb{R}^{n\times p}$, according to the definition, the covariance matrix of data set X can be expressed in the matrix product form:

$$\Sigma = \frac{1}{n-1}X^T X - \frac{1}{n(n-1)}X^T A X \tag{8}$$

where A is a $n \times n$ matrix with all elements equal to 1. The purpose is to find a transform operator T which will transfer the data matrix X to a modified data matrix $Y = XT$ and ensure that $\Sigma(Y)$ is a diagonal matrix.

$$\Sigma' = \frac{1}{n}Y^T Y - \frac{1}{n(n-1)}Y^T A Y = \frac{1}{n}T^T X^T T X - \frac{1}{n(n-1)}T^T X^T A X T \tag{9}$$

Perform singular value decomposition to the original covariance matrix Σ:

$$\Sigma = USV' \tag{10}$$

Define a squared diagonal matrix D_0 which contains n variance values of variables in X (the diagonal entries of the original

Factor	Distribution	Distribution parameters
U-234 content in graphite fuel(wt.%)	Normal	$\mu = 0.91,\ \sigma = 0.008$
U-235 content in graphite fuel(wt.%)	Normal	$\mu = 93.239,\ \sigma = 0.026$
U-236 content in graphite fuel(wt.%)	Normal	$\mu = 0.438,\ \sigma = 0.008$
U-238 content in graphite fuel(wt.%)	Balance	
O:U ratio in graphite fuel	Triangular	a=1.95, b=2.05, c=2
Graphite fuel B content (wt.%)	Normal	$\mu = 7.53,\ \sigma = 1.1619$
U mass content in fuel (wt.%)	Triangular	a=0.205, b=0.222, c=0.211
Density of graphite fuel (g/cm^3)	Triangular	a=1.71, b=1.76, c=1.73
Graphite fuel graphitization (%)	Triangular	a=58, b=60, c=59
C mass content in fuel (wt.%)	Balance	
Flat-to-flat distance of graphite fuel (in.)	Triangular	a=3.795, b=3.82, c=3.8
Standard fuel assembly outer radius (in.)	Triangular	a=3.935, b=3.985, c=3.96
Al 6063 composition (Non Al elements wt%)	Uniform	Details in ref [1] Table 3.17
Al 6063 composition (Al wt%)	Balance	
Al 6063 can thickness (in.)	Triangular (MCC)	a=0.05-1/64, b=0.05+1/64, c=0.05
	Uniform (SFA)	a=0.05-1/64/ $\sqrt{3}$, b=0.05+1/64/ $\sqrt{3}$
Zr-3 can thickness (in.)	Triangular (MCC)	a=0.025-1/64, b=0.025+1/64, c=0.025
	Uniform (SFA)	a=0.025-1/64/ $\sqrt{3}$, b=0.025+1/64/ $\sqrt{3}$

TABLE I. Variable and distribution information summary for TREAT uncertainty analysis, "MCC" stand for the TREAT minimum critical core model and "SFA" stand for the standard fuel assembly model

covariance matrix). Then define a new squared diagonal matrix $D \in \mathbb{R}^{n\times n}$, $D_{i,i} = \sqrt{\frac{D_{0i,i}}{S_{i,i}}}$. Therefore

$$D^{-1}U^T\Sigma V D^{T^{-1}} = D_0 \tag{11}$$

Also, since Σ is a symmetric matrix by definition, $U = V$ (when $m > n$). We have

$$D^{-1}U^T\Sigma U D^{T^{-1}} = D_0 \tag{12}$$

$$D^{-1}U^T\left(\frac{1}{n}X^TX - \frac{1}{n(n-1)}X^TAX\right)UD^{T^{-1}} = D_0 \tag{13}$$

Hence

$$T = UD^{T^{-1}} \tag{14}$$

In the case that X contains multivariate joint normally distributed variables, $Y = XT$ contains independent standard normal distributed variables.

This method works only when the covariance matrix of X is positive-definite. This is guaranteed by using a sample size which is large enough. It is known that when the random variables are close to independent from each other, the covariance matrix of X has full rank. In reality, when the sample size is large enough to produce convincing predictions, the covariance matrix of X is not ill-conditioned. This is a numerical observation and must be checked each time before transforming the raw matrix X to the factor samples desired. Notice that when the covariance matrix of X is ill-conditioned, for example, one or more of the Eigenvalues is zero, the matrix is not positive-definite. This operator fails in this case.

The operator T developed in this paper works only for joint-normal distribution. Hence it is only used to process the raw samples. Other desired distributions can be obtained through variable transformations on the post T processed samples.

III. RESULTS AND ANALYSIS

For TREAT standard fuel assembly SERPENT model, five groups of factors were considered. The groups include uranium vector, fuel composition, Al 6063 alloy composition, Al can thickness and Zr can thickness. For each factor (group), 150 samples were generated and tested. Another set of 300 samples which contain perturbations on all five groups of factors were studied. It was found that changes in uranium vector did not lead to a significant effect of the calculation results. Hence these two groups were not tested for the minimum critical core model. However, in the fuel composition group, boron contamination still remained as a significant uncertainty source and was kept for the minimum critical core study.

For the minimum critical core model, two geometry factors were added upon the factors studied for standard fuel assembly model. These two factors are the flat-to-flat distance of fuel block and the outer radius of the standard fuel assembly. All of the geometry factors studied are marked in the SERPENT model in Figure 2. 300 samples of perturbation on each factor alone were tested. To study the overall effect, another 600 samples which contain perturbations on all factors were tested. Notice that these sets of samples were repeated twice with the same raw data matrix. The first 600 samples

contain factor values transformed from the raw data matrix and the second 600 samples contain factor values transformed from the same raw data matrix but processed with the T factor before the transformation.

For all the sample sets, the covariance matrix of the raw data matrix were tested to be well-conditioned. Based on the law of large numbers, the average of the results obtained from a large number of trials should be close to the expected value. Hence, running average k_{eff} results for each factor (group) were plotted. The convergence of average k_{eff} with respect to the increasing sample size showed that the sample size was large enough.

The standard error of estimation of means and variances are calculated using the equations below:

$$\sigma_{\bar{x}} = \frac{S}{\sqrt{N}} \tag{15}$$

$$\sigma_{S^2} = S^2 \sqrt{\frac{2}{N-1}}. \tag{16}$$

Here S^2 denotes the variance of the results, S is the standard deviation.

Based on Equation 15 and 16 and the propagation of uncertainty, the standard errors of standard deviation estimation and relative uncertainty estimation are evaluated as:

$$\sigma_S = S \sqrt{\frac{1}{2(N-1)}} \tag{17}$$

$$\sigma_{\frac{S}{\bar{x}}} = \sqrt{\frac{1}{\bar{x}^2}\sigma_S + \frac{S^2}{\bar{x}^4}\sigma_{\bar{x}}} \tag{18}$$

1. Standard Fuel Assembly Model

The running k_{eff} average plots for each factor group are shown in Figure 3 and 4. The factors contained in the uranium vector group were not found to be significant sources of uncertainty. The sample size of $N = 150$ is more than enough for this group and the deviation among results was quite small. Factors in the Al6063 alloy composition group showed similar tendency. Zr can thickness and Al6063 can thickness were recognised as significant uncertainty contributors. Fuel composition group provided the most uncertainty as it contains the boron contamination factor. Due to the wide range of possible boron contamination in the graphite fuel, the k_{eff} value from standard fuel assembly model calculations varies by almost one percent.

Table II shows the same conclusions with more details. Notice that the overall uncertainty was about 300 pcm lower than the square root of the sum of all factor groups squared. This is expected since the sample size used for the all parameters included group was larger.

The reference calculation for a single standard fuel assembly model gives a k_eff value of 1.4117. Average k_{eff} results from the fuel composition, Al can thickness and Zr can thickness groups are shifted from the reference results. A shift like this usually has two reasons. The first reason is because

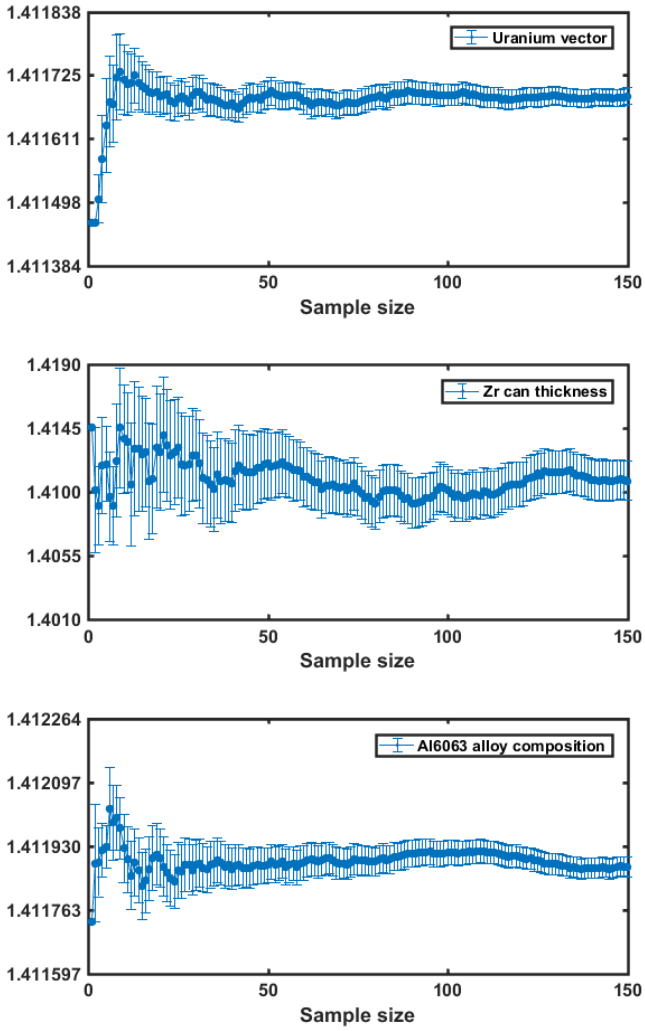

Fig. 3. Running average k_{eff} results for the standard fuel assembly model. Error bar in the plots shows the variation of the standard error of the mean value estimation with respect to the sample size.

Factor(s) perturbed	Sample size	Average k_{eff}	Relative uncertainty (pcm)
All parameters included	300	$1.4141 \pm 1.4125E-3$	1730.1 ± 70.8
Uranium vector	150	$1.4117 \pm 1.5052E-5$	13.1 ± 0.8
Fuel composition	150	$1.4108 \pm 1.3773E-3$	1195.7 ± 69.3
Al 6063 composition	150	$1.4119 \pm 2.5843E-5$	22.4 ± 1.3
Al can thickness	150	$1.4112 \pm 1.2498E-3$	1084.6 ± 62.8
Zr can thickness	150	$1.4127 \pm 1.2801E-3$	1109.8 ± 64.3

TABLE II. TREAT single standard fuel assembly model uncertainty analysis summary

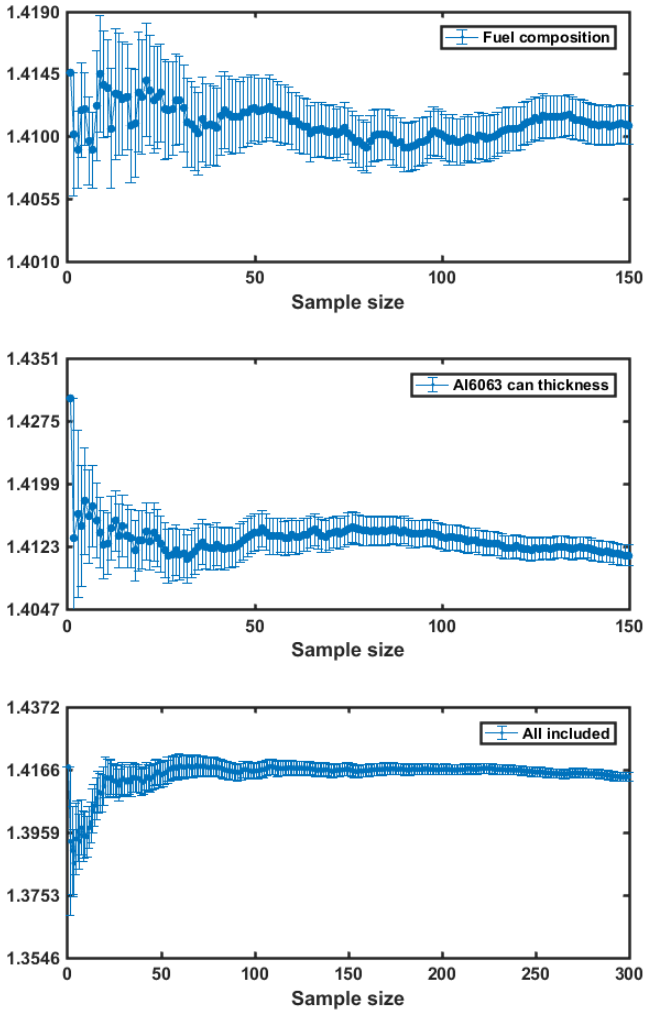

Fig. 4. Running average k_{eff} results for the standard fuel assembly model. The first two plots show single factor effects. The last one shows the overall effect of five factors on the k_{eff} estimation. Error bar in the plots shows the variation of the standard error of the mean value estimation with respect to the sample size.

of the covariance between perturbed factors or to be more general, the higher order responses of the joint probability distribution of factors. The second reason is the non-linearity of the model being studied. For Al can thickness and Zr can thickness factors, each set of samples contains single perturbed factor, hence there is no joint distribution or covariance. The shift should be resulted solely from the non-linearity of the model. Hence the linear assumptions widely used by direct perturbation method may not be appropriate when analysing uncertainties caused by geometry factors such as can thickness.

2. Minimum Critical Core Model

Based on the conclusions drawn from the standard fuel assembly model, the three material composition groups were discarded for minimum critical core uncertainty quantification study. Instead, boron contamination was used and flat-to-flat distance of fuel blocks and assembly outer radius were added.

The reference k_{eff} of minimum critical core model calculated with the Monte Carlo model is 1.0041.

Figure 5 and 6 plot the running k_{eff} average results of the minimum critical core model. Similar to the standard fuel assembly results, boron contamination, Zr can thickness and Al can thickness remained as significant factors. Flat-to-flat distance of fuel block caused observable variations among the k_{eff} values. It also provided the largest mean k_{eff} shift from the reference case. This is reasonable since perturbation on flat-to-flat distance of fuel block changes the amount of the fuel directly. The uncertainty caused by perturbations on outer radius of fuel assembly was almost negligible compared to the effect brought by the other factors.

The last plot in Figure 6 compares the sample set with/without T operator process. As shown in Table III, the process of removing "artificial" covariance caused about 70 pcm change in the relative uncertainty estimation.

In conclusion, the total uncertainty on the TREAT minimum critical core k_{eff} calculation at zero power caused by geometry factors and material composition is $\sim 1150 pcm$. The results presented in Ref. [1] was 495 pcm for the infinite lattice model of TREAT standard fuel assembly. Due to the difference in models and parameter distributions, it is hard to compare between these values. Based on the work presented in this paper, boron contamination and Zr can thickness were recognised as the most significant uncertainty sources of the

TREAT minimum critical core model. It was also found that the system had a non-linear response to some geometry factors such as the flat-to-flat distance of fuel block and Al can thickness.

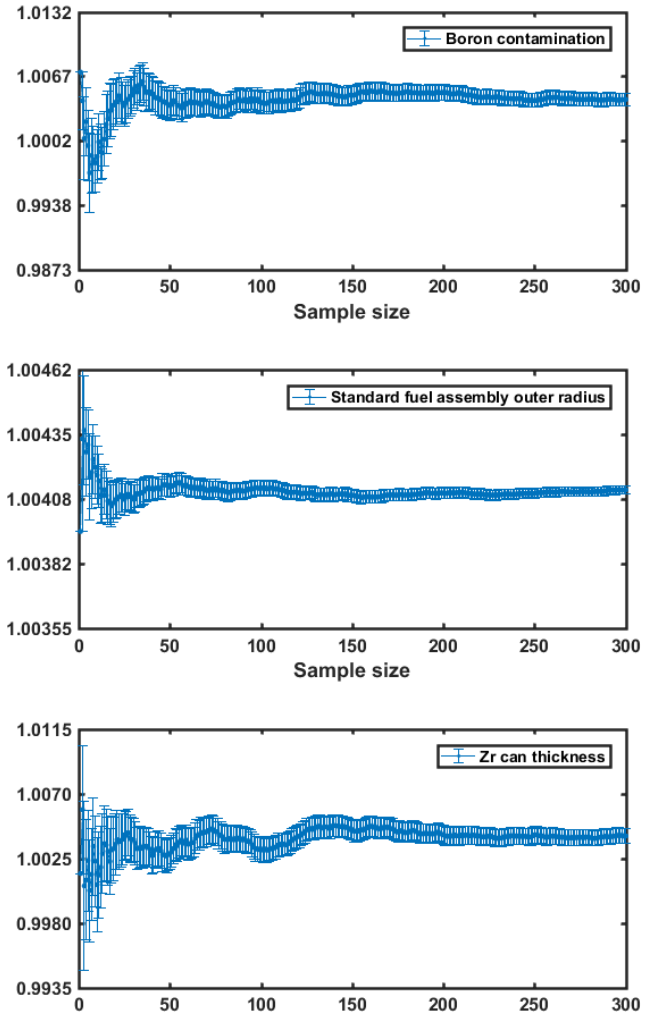

Fig. 5. Running average k_{eff} results for the minimum critical core model. Error bar in the plots shows the variation of the standard error of the mean value estimation with respect to the sample size.

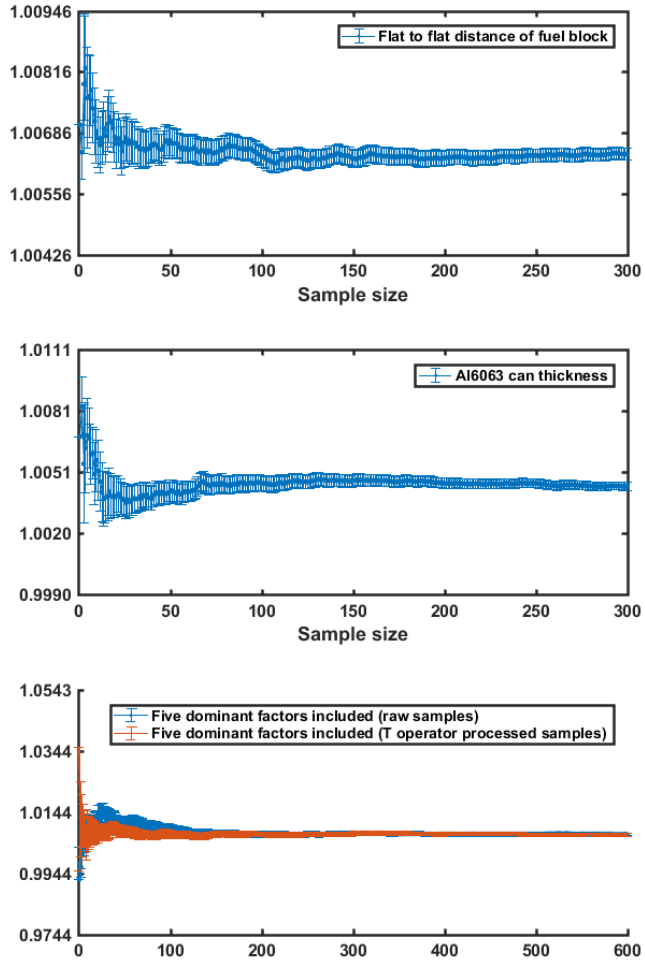

Fig. 6. Running average k_{eff} results for the minimum critical core model. The first two plots show single factor effects. The last one shows the overall effect of five factors on the k_{eff} estimation. Error bar in the plots shows the variation of the standard error of the mean value estimation with respect to the sample size.

IV. CONCLUSIONS

The work presented in this paper provides uncertainty analysis of the TREAT standard fuel assembly model and minimum critical core model. The distribution estimation and sampling method used were described in detail. Results showed that Boron contamination and geometry factors such as Zr can thickness, Al can thickness and flat-to-flat distance of fuel block were the most significant uncertainty contributors for these models. Because of the uncertainty in the boron contamination and the geometry factors, the relative uncertainty in

Factor(s) perturbed	Sample size	Average k_{eff}	Relative uncertainty (pcm)
All parameters included (raw)	600	$1.0070 \pm 4.9481E-4$	$1203.6 \pm 34.8pcm$
All parameters included (T operated)	600	$1.0068 \pm 4.6835E-4$	$1139.5 \pm 32.9pcm$
Boron content	300	$1.0044 \pm 6.3435E-4$	$1093.9 \pm 44.7pcm$
Flat to flat distance of fuel block	300	$1.0064 \pm 1.2939E-4$	$222.7 \pm 9.1pcm$
Standard fuel assembly outer radius	300	$1.0041 \pm 1.7732E-5$	$30.6 \pm 1.3pcm$
Al-6063 can thickness	300	$1.0044 \pm 1.9463E-4$	$335.6 \pm 13.7pcm$
Zr-3 can thickness	300	$1.0040 \pm 5.1837E-4$	$894.2 \pm 36.6pcm$

TABLE III. TREAT minimum critical core model uncertainty analysis summary

k_{eff} results for the minimum critical core may be higher than 1000 pcm. It was also shown that the model response to some geometry factors is non-linear and therefore methods based on linear assumption may not provide accurate predictions for this case.

V. ACKNOWLEDGMENTS

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