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Research Article

The Investigation of the Sensitivity of Monte Carlo Simulation Results to Modelling Approaches for Nuclear Reactor Cores

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Abstract

Monte Carlo simulations provide accurate results for the neutronic response of the system under consideration if modeling is performed appropriately since it has great influence on the results. Sensitivity analysis of modeling approaches for geometry and fissile material composition distributions in the reactor core was performed by taking ITU TRIGA Mark II Research Reactor into consideration. The method of defining fuel element positions in the core by using circular or hexagonal lattice was considered as one case and three different methods of lumping material compositions in the fuel elements were considered as another case since these approaches were used by deterministic codes hence the accuracy of deterministic codes were also investigated. The validation study showed that both MCNP and Serpent Monte Carlo codes resulted in good agreement with the experimental data with less than 1% relative error. It was observed that the handling of fuel composition in different ways did not influence the results significantly (up to 11.1 cents in reactivity). However, the influence of fuel arrangement is more pronounced (deviation in reactivity calculations is around 1$). These deviations at the results may affect the nuclear safety conclusion of reactors having small shutdown margins. It was also concluded that users of the deterministic codes should be aware of the fact that the simplifications in geometry and fuel composition in the core will result in significant deviation from the reality.

Keywords: Criticality, Monte Carlo, Neutronic Analysis, TRIGA Mark II, Serpent, MCNP, Geometrical Modeling, Fuel Composition Modeling.

Monte Carlo Simülasyon Sonuçlarının Nükleer Reaktör Kalp Modelleme Yaklaşımlarına Duyarlılığının Araştırılması

Öz

Monte Carlo benzetimleri, modelleme uygun şekilde yapılırsa söz konusu sistemin nötronik tepkisinin tahmininde doğru sonuçlar verir. Yakıt elemanlarında geometri ve bölünebilir malzeme bileşimlerinin dağılımının modellenmesinde kullanılabilecek yaklaşımların duyarlılığı İTÜ TRIGA Mark II Araştırma Reaktörü kullanılarak araştırılmıştır. Dairesel veya altıgen kafes kullanarak kalpteki yakıt elemanı konumlarını belirleme yöntemi bir durum, yakıt elemanlarındaki malzeme bileşimlerinin grup olarak toplanması için üç farklı yöntem diğer bir durum olarak değerlendirilmiştir. Böylece, sıklıkla bu yaklaşımları kullanan deterministik kodların da duyarlılığı araştırılmıştır. Doğrulama çalışması, hem MCNP 5 hem de Serpent 2 Monte Carlo kodlarının sonuçlarının %1'den az hata ile deneysel verilere iyi bir uyum sağladığını göstermiştir. Yakıt bileşiminin farklı şekillerde ele alınmasının sonuçları önemli ölçüde etkilemediği (reaktivitede maksimum 11,1 cent) gözlenmiştir. Ancak yakıt elemanı konum modelleme yaklaşımının etkisi daha belirgindir (reaktivitede maksimum 1 $). Sonuçlardaki bu sapmalar, küçük kapatma marjlarına sahip reaktörlerin nükleer güvenlik değerlendirmelerini etkileyebilir. Deterministik kodların kullanıcılarının, kalpteki geometri ve yakıt bileşimindeki basitleştirmelerin sonuçlarda önemli ölçüde sapmaya neden olacağı gerçeğinin farkında olması gerektiği sonucuna varılmıştır.

Anahtar Kelimeler: Kritiklik, Monte Carlo, Nötronik Analiz, TRIGA Mark II, Serpent, MCNP, Geometrik Modelleme, Yakıt Bileşimi Modellemesi.

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1. Introduction

Computational methods to model and simulate various phenomena taking place in nuclear reactors have become indispensable tools for developers in industry due to their extended capabilities with almost negligible cost as an alternative to complex and costly experiments. They are also important for the conceptual design studies and safety analyses for new reactors (Generation-IV) since it is impossible to demonstrate these analyses experimentally with currently available resources. For instance, core optimization for a sodium-cooled fast reactor was performed by using neutronic modelling to ensure an increase in neutron leakage in case of a core disruptive accident (Suetomi et al., 2017). In another study, it was concluded that lowering Zirconium content in the metallic fuel minimizes the excess reactivity of a compact linear burn-breed fast reactor after many different Zirconium region zoning have been analyzed numerically (Hartanto et al., 2016). In addition, a new fuel rod design parameters were defined for Super-Fast Reactor by conducting different numerical studies related to thermo-mechanical behavior (Ju et al., 2015). However, the main challenge for the utilization of these tools lies on verifying the accuracy and reliability in simulating the physical processes.

During the last decade, institutions having TRIGA Mark II type research reactors have adapted benchmark analyses in order to test the reliability of their simulations for further research activities (Khan et al., 2011; Tetsuo et al., 2011; Huda et al., 2004). It is known that the selection of engineering software codes, numerical techniques, and model development methodologies have significant importance on neutronic calculations. MCNP and Serpent performances for calculating the attenuation coefficient were compared by Ćalić et al. (2015) and slight differences have been found in the results especially for the reflector regions surrounding the core. Besides, a comparison between MCNP and TRIPOLI on calculating the multiplication factor for two different core configurations was presented by Henry et al. (2015) where Monte Carlo methodology showed a better performance than the deterministic approach in simulating the neutronic behavior. On the other hand, deterministic codes are proved to be less computational time demanding (Ivanov et al., 2016). Time requirements and the available computational power needed to simulate a physical phenomenon is always an issue. To that respect, several approaches are considered such as having an average fuel composition in the core, homogenizing the geometry, and reducing dimensions (Khan et al., 2011; Türkmen & Çolak, 2014; Rehman & Ahmad, 2018). The impact of applying geometrical homogenization presented by Wang et al., (2014) showed the negative impact of homogenization on accuracy of the multiplication factor calculations.

This study aims to investigate and reveal influence of modelling approaches on the results of Monte Carlo neutronic simulations for ITU TRIGA Mark II Research Reactor. MCNP 5 and Serpent 2 Monte Carlo simulation codes were utilized for the same problems to make comparison. This study has been performed to highlight whether there is a significant difference observed in results if some simplifications are taken into account regarding the geometrical modelling and fuel compositions. There are various ways to model reactor core with Monte Carlo codes. They usually allow users to use repeated structures in hexagonal or circular geometry for core modeling to reduce the modeling effort. In addition, fuel element compositions can be defined individually or can be taken the same if there is only a slight variation in fissile content. All these options have been analyzed and a comparison matrix was generated based on the results of two well-known Monte Carlo codes.

2. Material and Method

2.1. ITU TRIGA Mark II Research Reactor

ITU TRIGA Mark II is a 250 kW pool type research reactor owned by the Energy Institute of Istanbul Technical University. The reactor was commissioned in 1979 for research and education purposes to demonstrate both steady state and pulse mode operations. Reactor core is arranged to have 5 rings B to F around the central thimble to provide 90 positions in total for the placement of different elements. In ITU TRIGA Mark II research reactor, 69 positions are occupied by fuel elements and 16 positions are occupied by graphite dummy elements as seen in Figure 1. There are 3 control rods in the core namely transient, safety, and regulating. Safety rod is used for coarse reactivity adjustment while the regulating rod is used for multiplication factor tuning. Transient rod is used for power pulses. Pneumatic system in the F ring is used for quick irradiations and one position is reserved for neutron source in F ring. Inside the stainless steel clad, there are central zirconium rod, fuel meat which is a homogenized mixture of uranium (U) and zirconium hydride ($ZrH_{1.6}$) containing 8.45 wt.% enriched uranium having no more than 20% ^{235}U, and top and bottom graphite reflectors. The end fittings are also made of stainless steel. The graphite dummies that do not contain fuel and zirconium rod have similar geometry but have aluminum cladding.

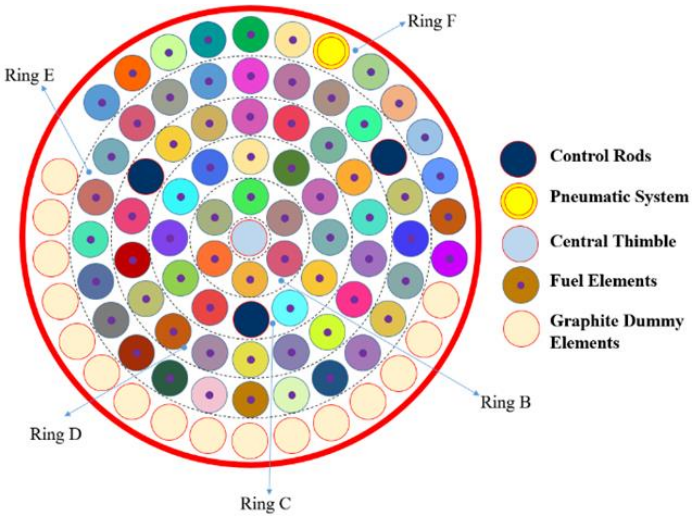

Figure 1. Cross-sectional view of ITU TRIGA Mark II Research Reactor

2.2. Problem Definition

For criticality calculations, simplifications that are made in geometrical configurations and/or material compositions such as homogenization are likely to cause the loss of information due to change on neutron leakage which is mathematically due to geometrical and material buckling. It was shown by Dall'Osso (2002) that changing the buckling value results in change of decay constant. It is emphasized by Yamamoto (2012) that there is a need for neutron leakage corrections in numerical modelling methods for both deterministic and Monte Carlo based methods when it comes to buckling search and introduced a leakage models for symmetric systems. Unfortunately, these models are

not valid for asymmetric cores such as the one in ITU TRIGA Mark II research reactor as seen in Figure 1. A new leakage model was described for asymmetric core buckling calculation by Yamamoto et al., (2018). Furthermore, a heterogeneous leakage model was presented by introducing three different schemes for PWR core which resulted in more accurate results than the homogenous model (Li et al., 2017). With such models, geometry can be simplified from 3D to 2D or 1D (Sohrabpour & Ezzati, 2009). However, these models require further development and they are complicated for implementation. In this study, the focus is not directly on buckling but on neutronic behavior represented by multiplication factor since a change in multiplication factor as a result of changes in geometrical modelling and material composition eventually indicates change in buckling value.

Six different cases, having different combinations of geometrical modelling and fuel compositions, have been selected for this study as seen in Table 1. For Model-1 and Model-4, all fuel element compositions were defined individually. For Model-2 and Model-5, the element compositions for each ring that are shown in Figure 1 was reduced to 3 totaling 15 fuel element compositions in the core. Each ring in core was assumed to have three distinct fuel compositions that is the minimum, the maximum, and ring averaged enrichment of that particular ring. For Model-3 and Model-6, all 69 fuel elements in the core were assumed to have one fuel composition which is the core average value.

Table 1. Model definitions used in the study

Geometry Arrangement	**The Number of Fuel Element Composition Defined in the Core**		
	69	**15**	**1**
Circular	Model-1	Model-2	Model-3
Hexagonal	Model-4	Model-5	Model-6

Cross sectional views from Model-1 to Model-6 generated with MCNP and Serpent codes are shown in Figure 2 and Figure 3. In these figures, each colour allocation in fuel elements represents different fuel enrichment. In these models, the circular arrangement represents exact position of each fuel element. On the other hand, hexagonal arrangement was created by using repeated structure option of the software under consideration. It is usually preferred due to simplicity and deterministic codes usually uses this method to model the core that has circular arrangement. Similarly, homogenized or uniform composition for fuel elements may be preferred due to simplicity and this method is used for some deterministic codes as well.

Monte-Carlo based codes MCNP 5 (Argonne National Laboratory, 2003) and Serpent 2 (Leppänen et al., 2015) were used for simulations. MCNP 5 and Serpent 2 have great capabilities in general geometrical and 3D modelling and can replicate the transport phenomena using continuous-energy cross sections which make them very suitable for the purposes of this study.

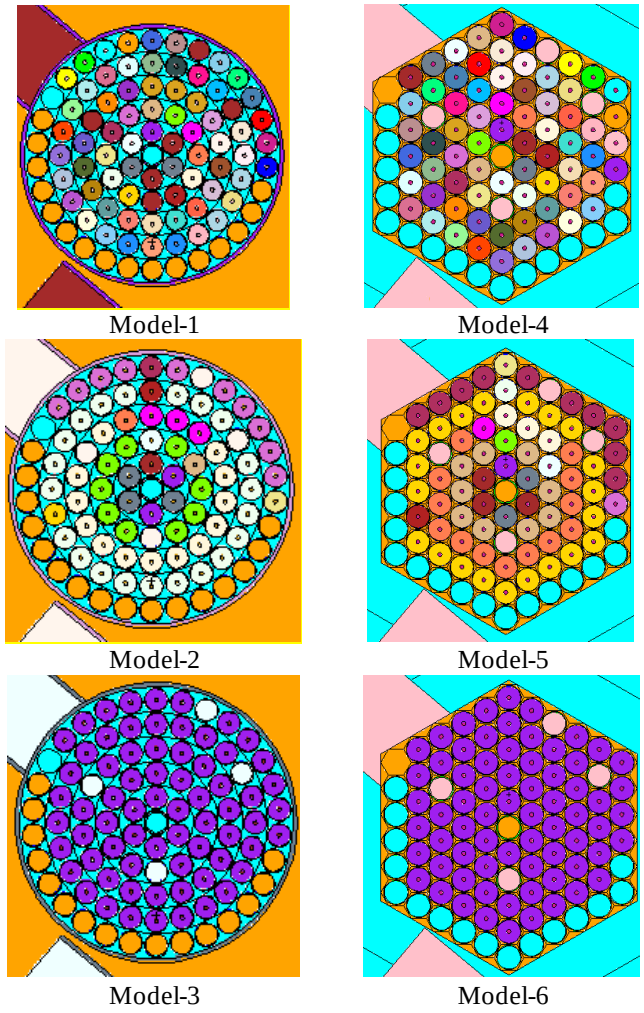

Figure 2. Cross sectional view of each model developed using MCNP 5 code

The details of the reactor such as grid plates, beam ports, central thimble, thermal column, reflector, aluminum tank, and concrete structure around the tank were included in the geometric models. For Model-1, -2, and -3 in MCNP 5 (Figure 2), all positions in the core were modeled individually and moved to their position with transformation card since MCNP 5 does not have circular lattice feature. For Model-4, -5, and -6, hexagonal lattice feature of the MCNP 5 code was used to place the fuel elements in their respective positions in the core. For these models, pitch between the fuel elements were used to calculate the dimensions of the hexagonal lattice cells, then, equivalent hexagons were generated for reflector and cavity regions. The cross-section library used for MCNP 5 is ENDF/VI.5 which considers delayed neutrons. In addition, neutron inelastic scattering S(α,β) interactions have been considered by taking the data from TMCCS library. Hence, the molecular binding effects of light water, graphite, hydrogen, and zirconium in $UZrH_{1.6}$ were evaluated at 300 K. Similarly, Serpent 2 has been used to model the same cores. However, unlike MCNP, a circular array cluster is possible with Serpent 2 therefore a cluster was defined to describe the 90 positions in the core for Model-1, -2, and -3. For Model-4, -5, and -6, similar to MCNP-5 code, hexagonal lattice was adopted (Figure 3). The cross-section library JEFF-3.1 has been used in Serpent 2 simulations. Meanwhile, the neutron inelastic scattering S(α,β) data were taken from JEFF-3.2 library.

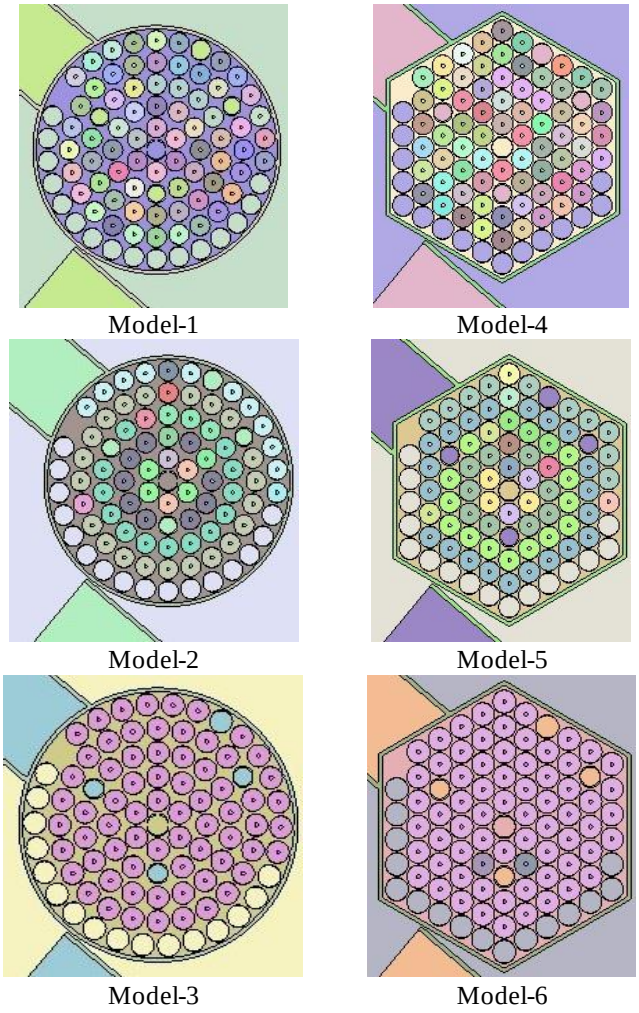

Figure 3. Cross sectional view of each model developed using Serpent 2 code

3. Results and Discussion

3.1. Benchmark Analysis

The benchmark analyses have been performed to verify the MCNP 5 and Serpent 2 reactor models generated for this study. The purpose of this benchmark analysis was to calculate the excess reactivity of the core with both codes and compare it against the experimental data from safety analysis report of the ITU reactor (General Atomics, 1979). Therefore, the results of Model-1 for both codes were benchmarked. All the Monte Carlo calculations have been performed with 1000 active cycles with 40000 neutrons per cycle.

The excess reactivity is determined by calculating the reactivity required from the insertion of each control rod to bring the reactor into the critical state (Asuku et al., 2015). Reactivity (ρ) is determined using the formula described in Eq.1. where $k_{eff,0}$ and $k_{eff,1}$ are the multiplication factor of consecutive states (Lamarsh & Baratta, 2001).

$$|\rho| = \frac{k_{eff,1} - k_{eff,0}}{k_{eff,1}} \quad (1)$$

In order to perform benchmark analysis, two states were simulated; in the first one, the reactor made critical by using control rods and in the second one, the reactor was super critical due to control rod movement. The resulting core excess reactivity values that are shown in Table 2 were calculated by using Eq. 1 for both codes. As seen in Table 2, both codes have shown good agreement with the experimental data since the results have less than 1% error. Therefore, the benchmark study verified the modeling and the input data and deck.

Table 2. Comparison between experimental and the calculated excess reactivity values

Experimental ($)	MCNP ($)	Serpent ($)	% Error for MCNP 5	% Error for Serpent 2
3.0309	3.0192	3.0035	0.38	0.79

3.2. The Influence of Geometrical and Fuel Composition Modeling

In order to investigate the influence of geometrical and fuel composition modeling on core criticality k_{eff} hence reactivity, simulations of Model-1 through Model-6 have been performed with both codes with 1000 active cycles and 40000 neutrons per cycle and by assuming all control rods are out of the core. The resulting multiplication factor values have standard deviation of 2×10^{-4} for all cases performed with both codes. Model-1 results from both codes have been taken as reference values since they represent the real core configuration without any simplification in geometry and material composition.

Results in Table 3 shows that models employing hexagonal lattice (Model-1, -2, and -3) results in higher values of reactivity. This increase is on the order of 30% for MCNCP 5 and 28% for Serpent 2. This is due to the fact that when the fuel elements are positioned at the center of the equivalent hexagonal cells, the distance between two fuel elements (pitch) became smaller. As a result, more compact core is situated and reactivity in the core increases.

Table 3. Calculated reactivity values for six models using MCNP 5 and Serpent 2

Model #	MCNP 5 Reactivity ($)	Serpent 2 Reactivity ($)
1	3.40	3.24
2	3.38	3.21
3	3.29	3.13
4	4.46	4.15
5	4.43	4.13
6	4.26	3.95

In addition, Table 3 shows that if the core is assumed to have only one average fuel composition (Model-3), the reactivity deviates around 4.2% for both codes from the reference case (Model-1) and if 15 different fuel element compositions are used in the core (Model-2), the results show around 0.6% deviation for both codes although the amount of ^{235}U in the core is the same in all models.

It is seen that there is not much difference in reactivity if each ring is lumped by using 3 different compositions (maximum, minimum, and the average of the rest in the particular ring). Almost all fuel elements in ITU TRIGA core have different enrichment therefore when the lumping is used, ^{235}U content increases in some fuel elements and decreases in others. The decrease is significant for high ^{235}U content fuel elements. Since

high ^{235}U content fuel elements are positioned close to the core center, the reduction in their ^{235}U content due to lumping causes decrease in reactivity.

It is important to point out that the reactivity difference with respect to Model-1 varies from -0.02 to 1.06 $ for MCNP 5 code, while from -0.03 to 0.91 $ for Serpent 2 code. When the shutdown margin value of ITU TRIGA reactor was considered, the decision on the safety of the reactor will be erroneous with 10% to 500% error. Therefore, the results of codes that are using Monte Carlo or deterministic methods must be used carefully.

The reactivity results in Table 3 also shows the different responses of each code. For each case, MCNP 5 overestimates the reactivity value by approximately 6% compared to Serpent 2. The difference between the cylindrical core and hexagonal core is more pronounced with MCNP 5 simulations since the deviation is around 30% for MCNP 5 and around 26% for Serpent 2. Therefore, MCNP code simulations are clearly more sensitive to the implemented geometrical modeling approach than Serpent 2 code. It should be noted here that on the contrary to Serpent 2, MCNP 5 does not have cylindrical lattice feature, therefore, TRIGA core geometrical modelling was performed by coordinate transformation. The same conclusions cannot be made for their response to fuel composition models. Both codes resulted in 0.8% deviation for reduction of fuel element compositions from 69 to 15 and 3.3% deviation when full core averaging of fuel composition is applied. Average of 6% difference between the results of MCNP and Serpent codes can be related to the fact that both codes utilize different nuclear data library. There are also computational uncertainties related to the simulation scheme which may influence the error buildup such as geometric modelling (defining lattices for core), source sampling (MCNP requires position of initial source locations, while Serpent initiates source randomly, which also results into more computation time in the latter), and numerical tolerance difference (surface transformation's matrix coefficients).

There are several studies in the literature about the comparison of Monte Carlo and deterministic codes. In general, simplifications in geometry and material compositions are used for deterministic codes. Sadewo et al. (2019) performed the comparison of WIMS and MCNP codes for Kartini TRIGA reactor. It was found that an average difference of 1.8% exists among code results for excess reactivity. Similarly, Rabir et al. (2012) reported 1.9% difference between TRIGLAV and MCNP code reactivity results. Criticality safety analysis for spent fuel pit of J. Stefan Institute TRIGA reactor was performed with MCNP and WIMS code by Ravnik et al. (1994). The reactivity results indicated 1.7% difference. The novelty of this study comes from the fact that modeling difference was investigated by using the same code. The literature presented above includes two different codes that use different calculation methodology and modeling approaches. Therefore, it is difficult to point out the reason of the difference in the results.

4. Conclusions and Recommendations

Monte Carlo simulations of ITU TRIGA Mark II Research Reactor have been performed by using MCNP 5 and Serpent 2 codes to investigate the effect of different approaches in modeling, specifically in geometry and fuel composition, on neutronic parameters. The benchmark analysis validated the simulation geometry and selected simulation parameters for both MCNP 5 and Serpent 2 models since the results showed good agreement with the experimental data with relative errors less than 1%.

Six models have been defined to investigate the influence of different geometry and fuel composition modeling approaches on core excess reactivity value. It has been found that reactivity drops in the same rate with fuel element composition simplification regardless of the code utilized (0.8% for 69 fuel compositions to 15 and 3.3% for 69 fuel compositions to one, respectively). In addition, this drop becomes more pronounced at very high level of homogenization i.e. only one fuel composition to represent all fuel elements. Geometric transformation from circular to hexagonal lattice has induced more deviation than what is produced by averaging the fuel composition to simplify the simulations (around 30%). It may be concluded that MCNP 5 code is more sensitive to the modeling approaches since the deviation in case of MCNP 5 model reaches up to 1.06 $ while in case of Serpent 2 it reaches up to 0.91 $. For reactor with small shutdown margin, inappropriate modeling may affect the conclusion about the safety of the reactor.

The need for simplification in simulations is sometimes inevitable due to limited computational capacity, time restrictions, complexity of the design, and missing details. Furthermore, it might be needed for the purpose of suggesting new technology or concepts that are very expensive to be experimented or established. The investigation which is presented in this study gives a valuable insight on how the numerical results would be influenced by adapting such approaches, in other words, when these influences are considered negligible and when they are too significant to be ignored. This insight also helps to understand how to treat the results of deterministic codes which use fuel homogenization and hexagonal lattice for ring type core configuration.

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