Application of CNUREAS and MCNP5 Codes to VVER-1000 MOX Core Computational Benchmark

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ABSTRACT

In order to strengthen the nuclear design calculation capacity in Turkey, CNUREAS (Cekmece Nuclear Reactor System) was developed to provide easy usage of neutronic and thermal hydraulic nuclear codes included in the CNUREAS package. It was tested and used for research reactors and PWR type power reactors. Modifications were performed to add hexagonal geometry support taking into account VVER type reactors employing hexagonal fuel assemblies that will be built in Turkey. "VVER-1000 MOX Core Computational Benchmark" was used to test new features of the CNUREAS. The maximum deviation in effective multiplication factor results of CNUREAS was 0.7% with deterministic codes and 1.5% with Monte Carlo codes. It was concluded that CNUREAS can be used for neutronic calculations of VVER type power reactors with appropriate cross section libraries and deterministic and Monte Carlo techniques give comparable results when both provided with appropriate cross section libraries.

Keywords: CNUREAS, MCNP5, VVER-1000, MOX

1 INTRODUCTION

Strengthening calculation capabilities of countries embarking on nuclear power has a vital importance. Some of those calculations involve neutronic codes such as WIMS-ANL (Deen et al., 2000) and CITATION (Fowler et al., 1971) and thermo-hydraulics codes such as PARET (Woodruff et al., 2001), COBRA (Wheeler et al., 1976), TRANSV2 (Klein et al., 1989), and RELAP5 (Siefken et al., 2001). Generally, a lot of effort is required for input preparation and data transfer from output of one code to input of other code. In order to make those codes available to users from most experienced to beginners, CNUREAS (Cekmece Nuclear Reactor System) (Erdogan, 2008) was developed. CNUREAS is a graphical user interface developed in Cekmece Nuclear Research and Training Center in order to create and control the input and output of the above mentioned nuclear codes. CNUREAS hides these underlying nuclear codes from the user by converting the user specified information into the format required by them therefore simplifying the overall operation. Furthermore, the amount of data requested is minimized since CNUREAS performs necessary intermediary calculations. Results are presented in computer graphics and color maps so as to provide the user with the means to process them fast and effectively.

Performing assembly and core neutronic benchmark problems is a good way to start building up calculation capacity and to validate CNUREAS code. CNUREAS has already been tested and used for calculations related with pool type TR-2 research reactor which is situated in Cekmece Research and Training Center and PWR type power reactors. In the near future, Turkey is going to have VVER type reactors that have hexagonal fuel assemblies. Therefore it is necessary to make adjustments in CNUREAS to model and run problems having hexagonal geometry. Several modifications were performed and benchmarks involving VVER type reactors were used to test and validate CNUREAS. One of those benchmark problems is "VVER-1000 MOX Core Computational Benchmark" (Gomin et al., 2005) which is established by NEA. The benchmark investigates the physics of a whole VVER-

1000 reactor core using two-thirds low-enriched uranium (LEU) and one-third MOX fuel and it also contributes to the computer code certification process and calculation method verification process. A total of three solutions were submitted from two countries with each participant using different methods and nuclear data combinations. Two of the solutions are based on continuous energy Monte Carlo methods (MCNP4C (RSICC, 2000) and MCU (Kalugin et al., 2014)), while the other solution is based on collision probability (or similar) method (RADAR). Thilagam et al. (2009) performed same calculations with different codes and Thilagam et al. (2010) used benchmark results to perform inter comparison of evaluated data.

In this study, CNUREAS and MCNP5 (X-5, 2003) codes were employed to analyze VVER-1000 MOX core Computational Benchmark. The results are compared with benchmark results not only to make sure that CNUREAS passes the data from user to codes correctly so as to generate geometry and outputs but also to check the integrity of exchange of data form one code to another. In addition, deterministic and probabilistic approaches were compared.

2 VVER-1000 MOX Core Computational Benchmark

The benchmark model consists of a full-size 2-D VVER-1000 core with heterogeneous 30% MOX-fuel loading. The system basically consists of fuel assemblies and a reflector. Twenty-eight assemblies in 60^o rotation symmetry angles are considered as seen in Figure 1. The system has an infinite axial dimension and vacuum condition on the side surface. The core consists of fresh and burned fuel assemblies (FA) of graded UOX FA with U-Gd burnable absorber (BA) rods as seen in Figure 2 and graded, profiled MOX FA with U-Gd BA rods as seen in Figure 3. Fuel materials have isotopic composition according to assembly burn-up. A reflector consists of the following elements ordered from center to periphery: water gap, steel buffer with water holes, steel barrel, downcomer (water) and steel vessel as seen in Figure 4. Six different state calculations were performed. The reactor state is described by material temperatures and the presence of absorber rods in the core. These states are described in Table 1. For each state k_{eff} (effective multiplication factor), assembly average fission reaction rate distribution for the 28 assemblies in the core, and cell average fission reaction rate distribution within several assemblies (3, 21, and 27, see Figure 1) for 331 cells per each of the three assemblies for state 1 are requested from participants. The other detail of the core geometry and isotopic compositions of the fuel materials, fuel cladding, central and guide tubes, absorber cladding, absorber rod, steel buffer, steel barrel, and steel vessel are presented in Gomin et al. (2005).

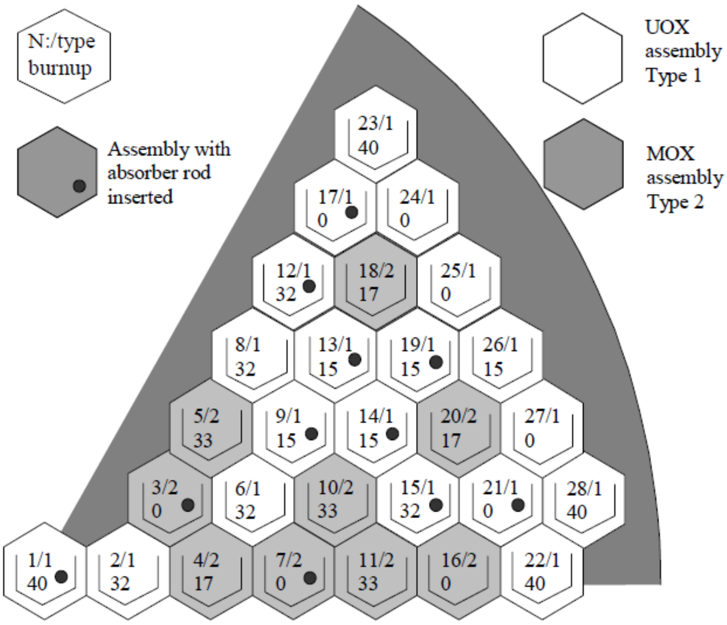

Figure 1 Pattern of the VVER-1000 core with 30% MOX fuel loading.

Table 1 Reactor state descriptions.

State	**State name**	**Fuel T, K**	**Moderator in FA T, K**	**Moderator in FA material**	**Reflector T, K**	**Water gap, water hole, downcomer material**	**Absorber rod**
S1	Working state	1027	575	M575B1.3	560	M560B1.3	-
S2	State with constant temperature	575	575	M575B1.3	560	M560B1.3	-
S3	Cold state with high boron content	300	300	M300B2.8	300	M300B2.8	-
S4	Working state without boron	1027	575	M575B0	560	M560B0	-
S5	State with constant temperature 1without boron	575	575	M575B0	560	M560B0	-
S6	State with control rods inserted	553	553	M553BO	553	M553BO	Inserted

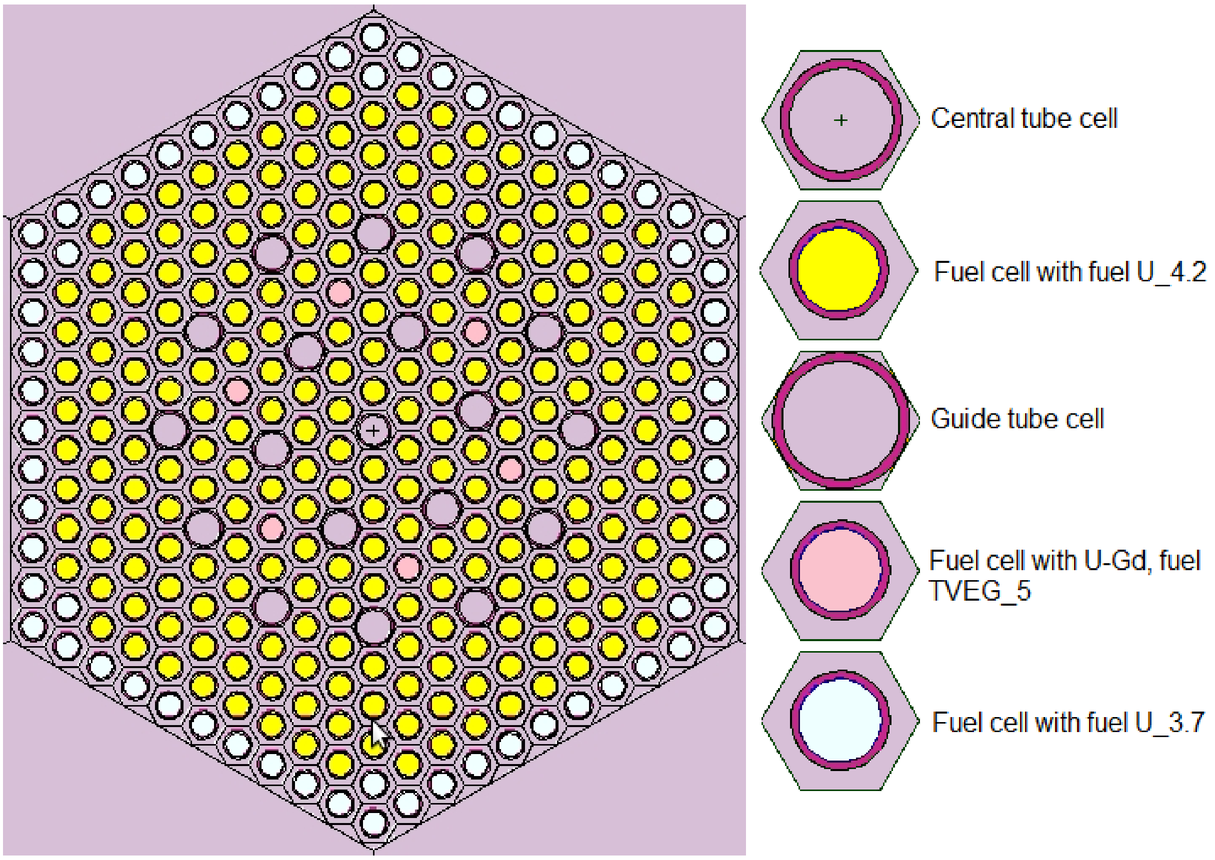

Figure 2 Pattern of graded UOX fuel assembly (MCNP5 model).

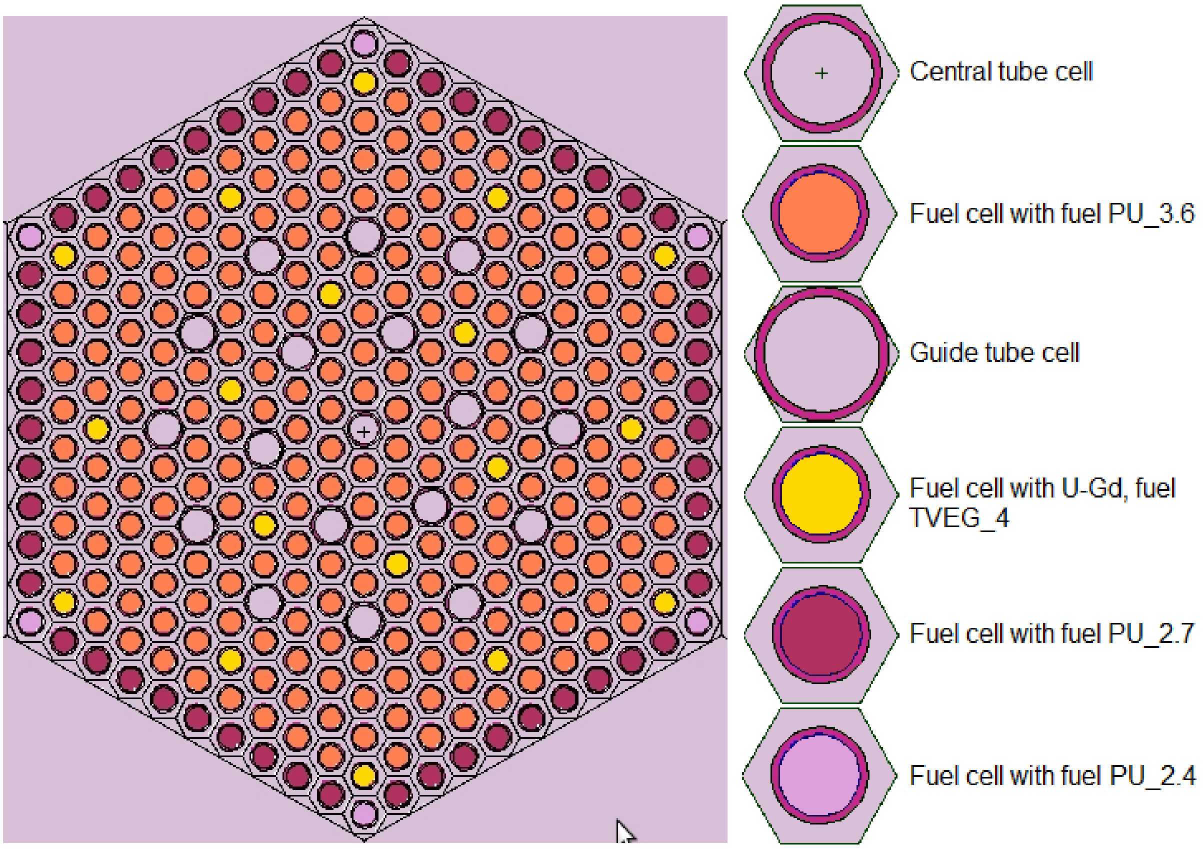

Figure 3 Pattern of graded MOX fuel assembly (MCNP5 model).

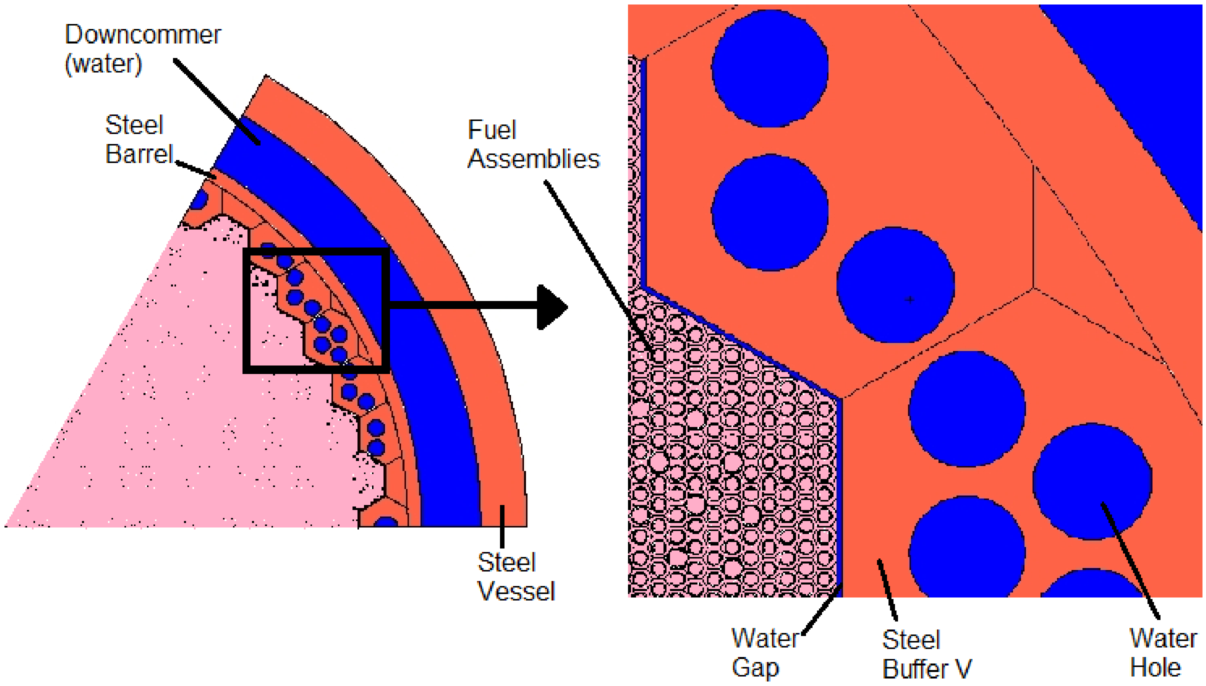

Figure 4 Location of different elements in the core (MCNP5 model).

3 Results and Discussion

The VVER-1000 MOX core shown in Figure 2 to Figure 4 was modeled with MCNP5 and CNUREAS and calculations were performed for 6 different states presented in Table 1. The full core was modeled with MCNP5 without any geometrical assumptions. CNUREAS modeling required a little bit of more effort since WIMS does not support hexagonal cell model. Therefore, FA cylindrical models having equivalent areas as hexagonal assemblies were generated as seen in Figure 5 and Figure 6. These FA were then used to generate core model for calculations as seen in Figure 7. In order to see the performance of WIMS with cylindrical assemblies, Assembly 25 in Figure 1 was selected and criticality calculations were performed with MCNP5 and WIMS. In MCNP model, reflected boundary condition was applied to make the results comparable. Results showed that kinf calculated by WIMS is about 3% higher compared to the results of MCNP5.

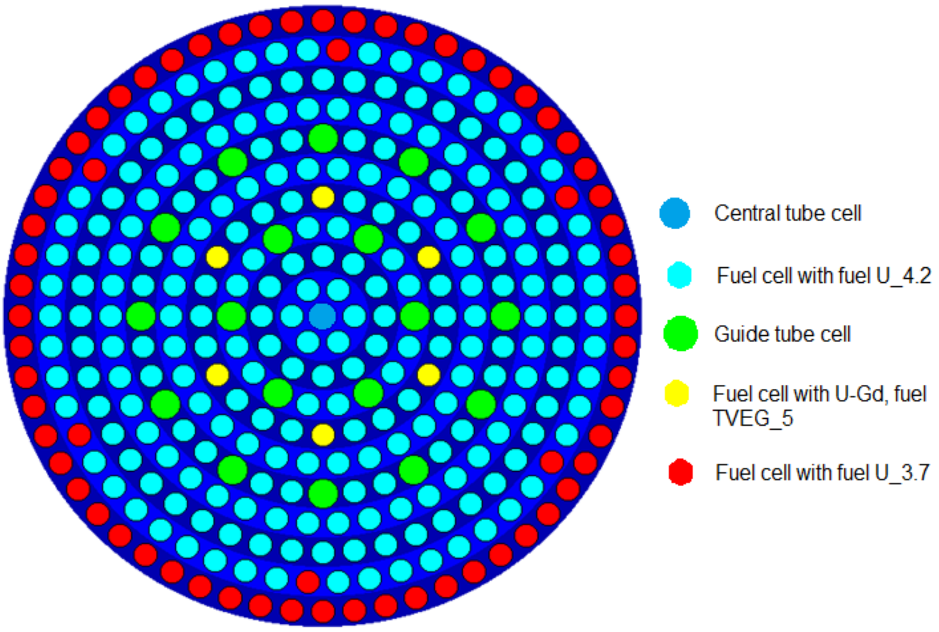

Figure 5 CNUREAS model of UOX FA.

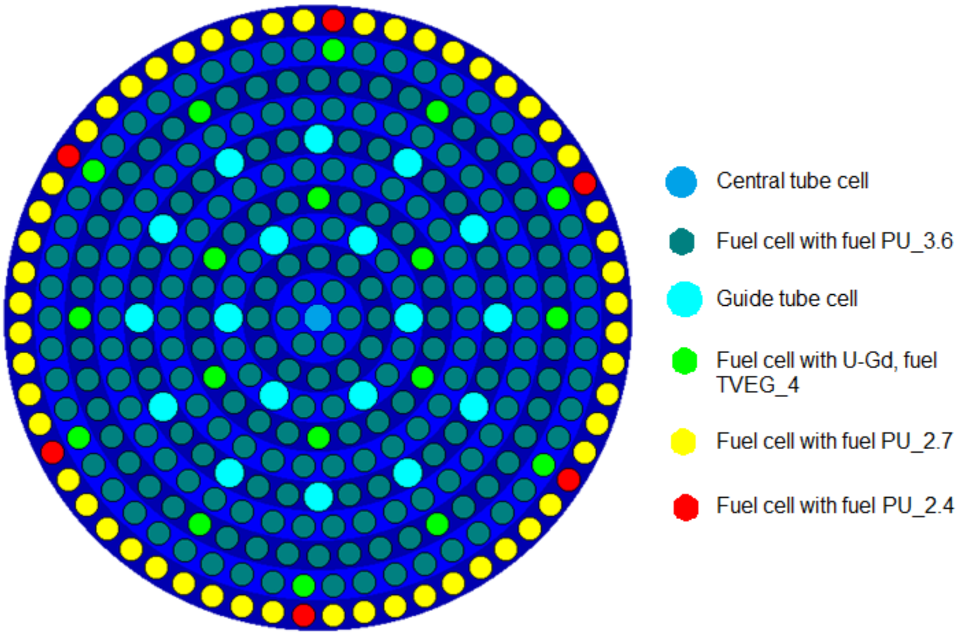

Figure 6 CNUREAS model of MOX FA.

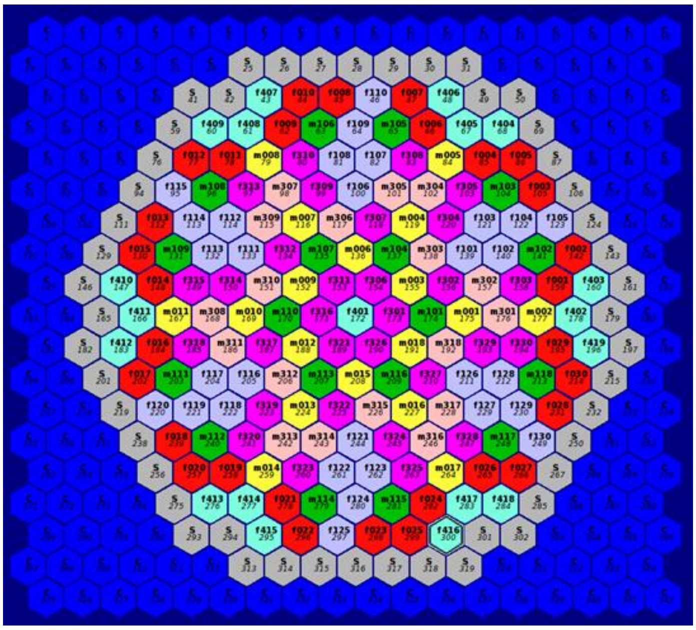

Figure 7 CNUREAS core model for state 1.

MCNP5 was used with 5000 active neutron production cycles with 20000 neutrons per cycle resulting total of 100×10^6 neutrons for state 1 and with 2000 active neutron production cycles with 20000 neutrons per cycle resulting total of 40×10^6 neutrons for other states to provide same simulation parameters with benchmark (Gomin et al., 2005). In the benchmark, 50 cycles were skipped for the simulation of state 1 and 500 cycles were skipped for other states. In order to determine the number of cycles to be skipped for MCNP5 calculations, convergence plots of Shannon entropy of fission source distribution (Brown et al., 2007) and k_{eff} were generated as seen in Figure 8. This convergence testing included not only k_{eff} but also Shannon entropy because it is known that Shannon entropy of fission source distribution converges more slowly than k_{eff} (Brown, 2006). It is seen in Figure 8 that for state 1 100 cycles and for state 2 150 cycles are required for convergence. It should be indicated at this point that convergence plots of state 3 to 6 are similar to state 2 therefore are not given here. For this study, 100 cycles for state 1 and 500 cycles for state 2 to 6 were skipped.

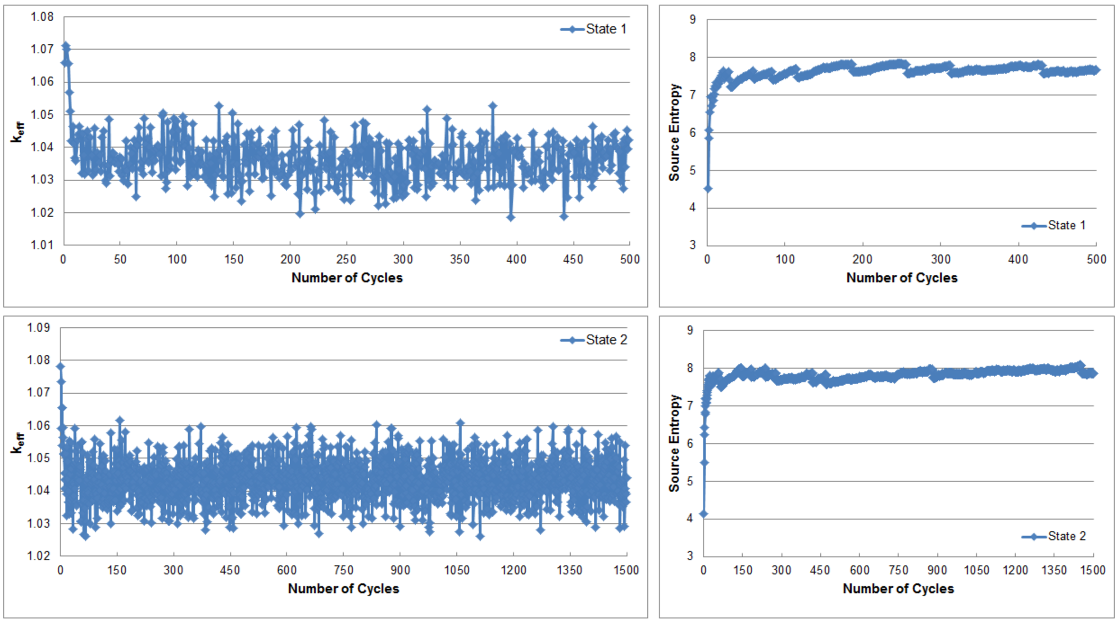

Figure 8 Convergence plots of Shannon entropy of fission source distribution and k_{eff} for state 1 and 2.

3.1 Effective multiplication factor k_{eff}

The simulation and calculation results from CNUREAS and MCNP5 together with benchmark results for all states in Table 1 are presented in Table 2. Table 2 indicates that MCNP5 results are very close to “Benchmark Mean” for every state since maximum difference is 0.8%. It is also seen that except state 3 MCNP5 underestimates k_{eff} results. When results of codes using Monte Carlo technique are analyzed it is seen that their results are also very close to each other since maximum difference is 0.9% with MCNP4C and 0.5% with MCU. MCNP5 results are systematically lower than MCNP4C results for all states. There isn’t any specific pattern when MCU results are considered. Since the method used in these codes is almost the same, the difference is probably because of the fact that different cross section libraries are utilized. MCNP5 uses ENDFB66, MCNP4C uses JEF2.2, and MCU uses MCUDAT2.1 cross section library for simulations.

Table 2 k_{eff} results of all reactor states.

State	MCNP5	Sigma (%)	CNUREAS	MCNP4C	Sigma (%)	MCU	Sigma (%)	RADAR	Benchmark Mean
S1	1.03614	0.007	1.03590	1.03770	0.007	1.03341	0.013	1.03769	1.03627
S2	1.04339	0.010	1.04550	1.05132	0.010	1.04719	0.012	1.05117	1.04989
S3	0.93397	0.011	0.93630	0.93416	0.010	0.93237	0.010	0.93204	0.93286
S4	1.13511	0.010	1.14960	1.13871	0.011	1.13390	0.012	1.14081	1.13781
S5	1.14333	0.010	1.16020	1.15400	0.010	1.14932	0.012	1.15574	1.15302
S6	1.03914	0.010	1.03270	1.04729	01011	1.04267	0.009	N/A	1.04498

When CNUREAS results are compared with “Benchmark Mean”, it is seen that maximum difference in k_{eff} is around 1.2%. This occurs at state 6 where absorber rods are inserted into the core. In spite of that, results of RADAR code which is also a deterministic code are consistent with CNUREAS since the maximum difference is 0.7%. The results are very close although cross section library used by RADAR is 63-group library with 40 thermal groups (with boundary energy of 1.0 eV) and by CNUREAS is ENDF/B-VI 69-group. In addition, there isn’t any specific pattern of overestimation or underestimation between CNUREAS and RADAR codes. It should be noted here that state 6 result of RADAR is not available in the benchmark. Therefore CNUREAS result of state 6 cannot be compared. In order to fully test the capability of CNUREAS code, the results of Thilagam et al. (2009) were used to evaluate CNUREAS result for state 6. The comparison revealed that the difference is around 2.5%. Since the results of Thilagam et al. (2009) are compatible with “Benchmark Mean” except state 6, it can be said that there could be limitations in diffusion theory codes when strong absorber exists in the system.

In general, results of CNUREAS and RADAR codes are in good agreement which is a very good indication that CNUREAS runs do not have any problems since both codes use similar calculation method. In addition, results of CNUREAS and Monte Carlo codes are in good harmony for states 1 to 3, differences arise when states without boron are simulated (state 4 and 5), and it is more pronounced when absorber rods are inserted into the core (state 6). These differences can be explained by usage of different methods and cross section libraries. As a result, it can be said that VVER-1000 MOX core is well generated by CNUREAS and there is not any problem related with inner data transfer and calculations performed by CNUREAS when modelling hexagonal geometry.

3.2 Assembly average fission reaction rates

Assembly average fission reaction rates and corresponding statistical uncertainty of the MOX cores having state 1 to 5 in Table 1 are presented in Figure 9 to Figure 13. It is reported in the benchmark that estimated statistical uncertainty of assembly average fission rates for state 1 is between 0.05-0.2 % for MCNP4C and 0.5-1.1 % for MCU. MCNP5 statistical uncertainty for the same state is between 0.07-0.2 %. For state 2 to 6, MCNP4C and MCU statistical uncertainties are between 0.1-0.3 % and

0.4-1.1 % while MCNP5 estimate of it is between 0.1-0.4 %. It should be noted here that fission reaction rate results from CNUREAS was not available for state 6. Therefore MCNP5 calculations were not performed either.

It is seen from the Figure 9 to Figure 13 that MCNP5 assembly average fission rates differ from the ”Benchmark Mean” fission rates as much as 13%. When MCNP5 results are compared with MCNP4C and MCU, the maximum difference is about 11%. This discrepancy between the different versions of MCNP can be explained by different set of cross section data used. It is worth noting here that MCNP4C and MCU results are very close to each other since the maximum difference in results is only 1.5%. Similarly, CNUREAS predicts assembly average fission rates with a maximum difference with ”Benchmark Mean” being 14%. The comparison between two deterministic codes reveals that there is maximum 15% difference between CNUREAS and RADAR results. In the benchmark, it is reported that computer codes using two different methods show very good harmony taking into account that maximum difference between codes is 3%. But, in this study, it is found that there is at least 20% difference in fission rate results of particular assemblies. The maximum difference occurs with MCNP5.

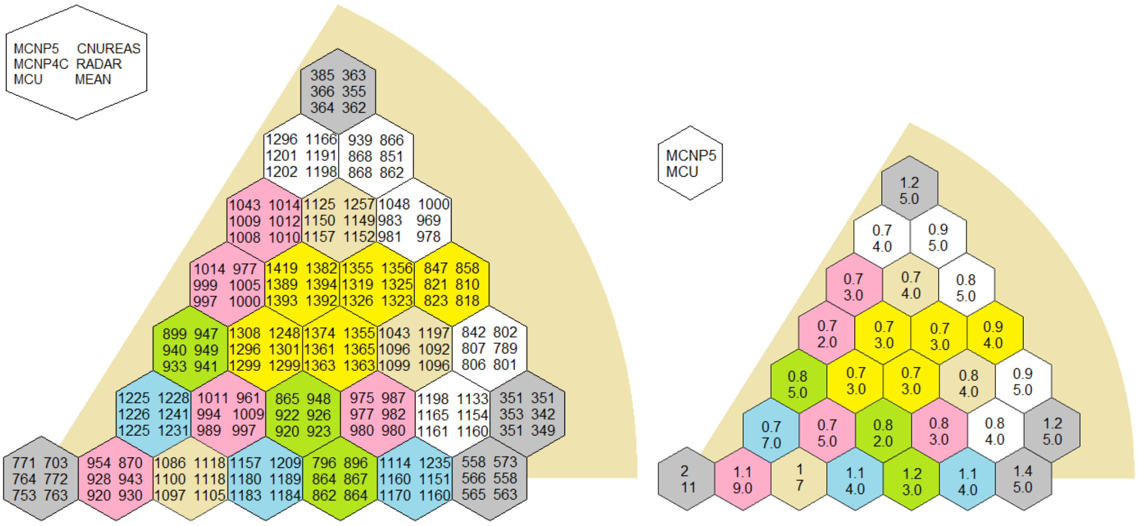

Figure 9 Assembly average fission reaction rates (x 100) and statistical uncertainty (0.1%) for state 1.

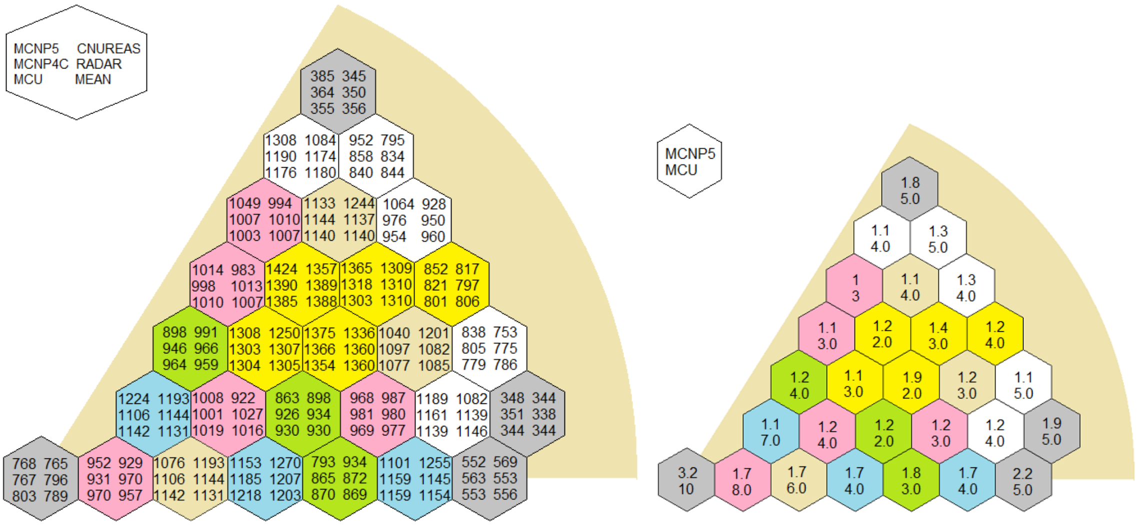

Figure 10 Assembly average fission reaction rates (x 100) and statistical uncertainty (0.1%) for state 2.

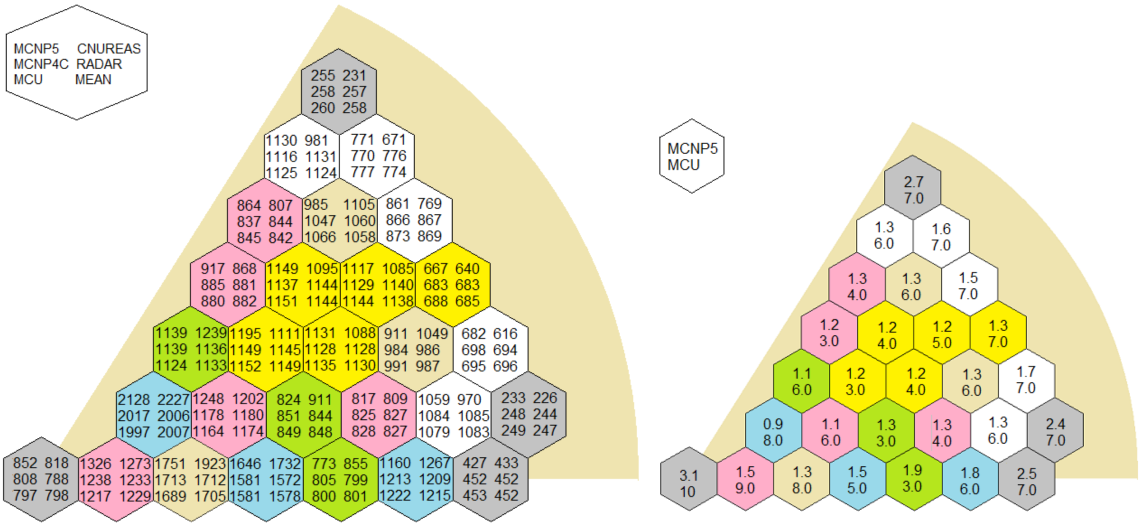

Figure 11 Assembly average fission reaction rates (x 100) and statistical uncertainty (0.1%) for state 3.

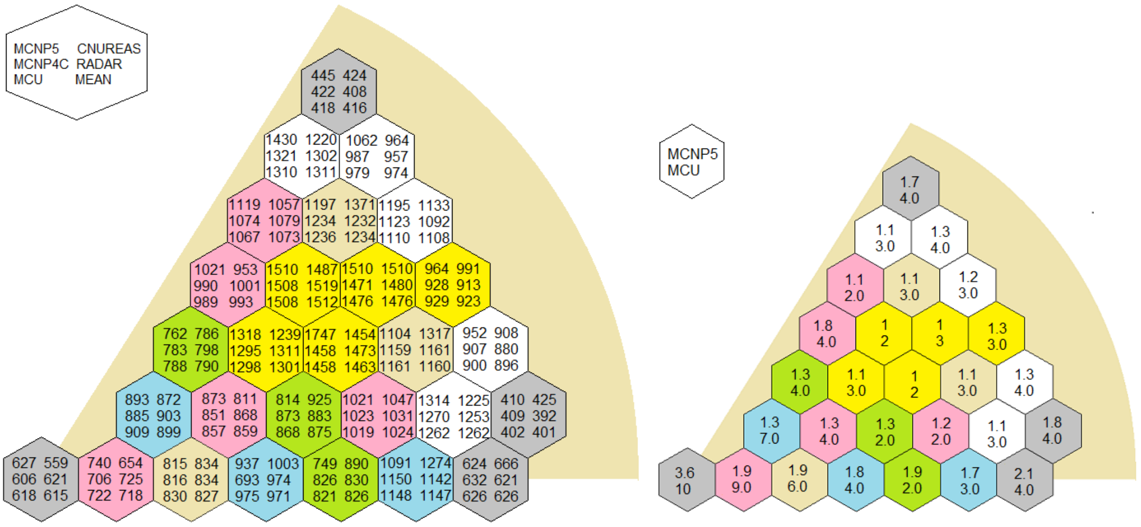

Figure 12 Assembly average fission reaction rates (x 100) and statistical uncertainty (0.1%) for state 4.

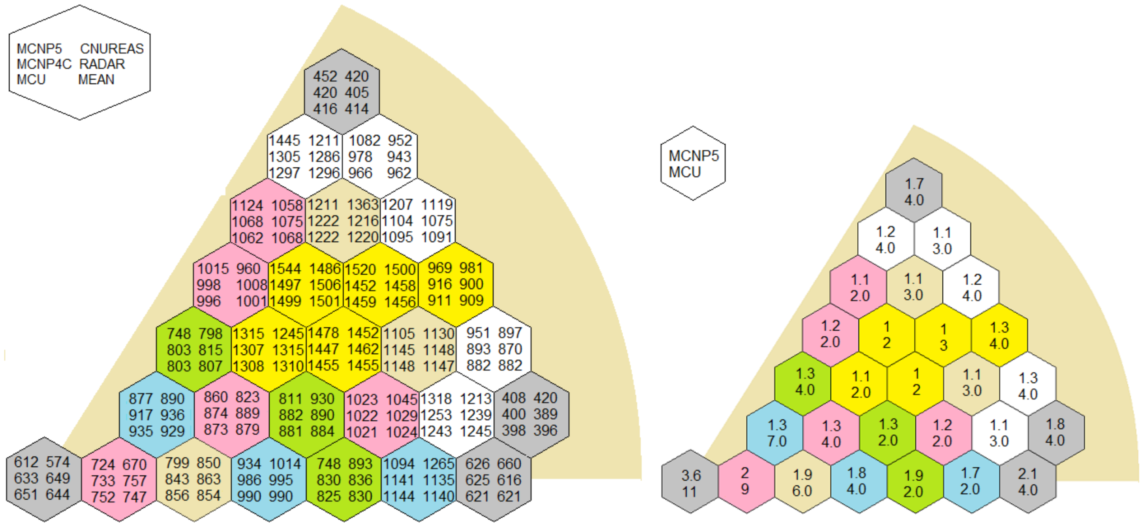

Figure 13 Assembly average fission reaction rates (x 100) and statistical uncertainty (0.1%) for state 5.

When the results is analyzed to see whether there is a systematic error in modeling and running the benchmark with CNUREAS, it is concluded that the difference between benchmark and CNUREAS results was independent of assembly position or assembly type (MOX or UOX). Therefore, it can be said that there is not any problem in modeling and running the problem with CNUREAS. Special attention must be on cross sections used since both MCNP5 and CNUREAS use generic cross section libraries generated for general use not for this specific problem.

4 Conclusions

CNUREAS code package developed to perform both neutronic and thermal hydraulic calculations for research and power reactors and modified to include hexagonal geometry modeling taking into account the fact that Turkey is going to have VVER type reactor which employs hexagonal fuel assemblies. The new version was tested by using VVER-1000 MOX Core Computational Benchmark and MCNP5. In addition, deterministic and Monte Carlo methods were compared.

It is seen that effective multiplication factor results of CNUREAS code have quantitative agreement with ”Benchmark Mean” and other deterministic code used in benchmark since the maximum deviation is 1.2% with benchmark mean and 0.7% with the deterministic code. Furthermore, its results are comparative with Monte Carlo code results maximum deviation being 1.5%. Differences arise when more detailed results like fission reaction rate of assemblies are examined. The maximum deviation is 13% with the deterministic code, 14% with “Benchmark mean”, and 20% with Monte Carlo codes. This is because of the generic cross section libraries used in CNUREAS and cylindrical modeling approach applied in WIMS. Similar result is also observed with MCNP5 which also uses generic cross section library. The effect of cross section library is not so pronounced for effective multiplication factor calculations since it is an overall core result.

In general, it can be said that modifications performed on CNUREAS to support hexagonal geometry are validated. There is no problem during the data transferring from graphical interface to codes running background, inner calculations performed by CNUREAS, and data transfer from output of one code to input of other code. CNUREAS with an appropriate cross section library can be used for VVER type power reactor calculations.

Acknowledgement

This research Project is supported by Turkish Atomic Energy Authority (Project Number: A1.H1.P2.03)

Notation

LEU	Low enriched uranium fuel
MOX	Mixed oxide fuel
FA	Fuel assembly
UOX	Fuel type containing Uranium
U_Gd	Uranium Gadolinium burnable absorber
k_{eff}	Effective multiplication factor
k_{inf}	Infinite multiplication factor
$U\_3.7$	Uranium fuel with ^{235}U enrichment 4.2% wt.
$TVEG\_5$	Uranium-gadolinium fuel with enrichment 3.3% wt. on ^{235}U and 5% wt. on Gd_2O_3
$PU\_3.6$	MOX fuel with fissile Plutonium isotopes enrichment 3.62% wt.
$TVEG\_4$	Uranium-gadolinium fuel with enrichment 3.6% wt. on ^{235}U and 4% wt. on Gd_2O_3
$PU\_2.7$	MOX fuel with fissile Plutonium isotopes enrichment 2.69% wt.
$PU\_2.4$	MOX fuel with fissile Plutonium isotopes enrichment 2.42% wt.

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