

Comparison of thorium nitride (ThN) and uranium nitride (UN) fuel on small modular PWR in neutronic analysis has been carried out. PWR in module is one type of reactor that can be utilized because of its small size so that it can be placed on demand. Neutronic calculations were performed using SRAC version 2006, the data library using JENDL 4.0. The first calculation was fuel pin (PIJ) calculation with hexagonal fuel pin cell type. And the second calculation was reactor core (CITATION) calculation using homogeneous and heterogeneous core configurations. ThN and UN fuels use heterogeneous configurations with 3 fuel variations. The reactor geometry was used in two fuels are the same, with diameter and height active core was 300 cm and 100 cm. In this research, Np-237 was added as a minor actinide in the UN fuel to reduce the amount of Np-237 in the world and also reduce the k-eff value. For ThN fuel, Pa-231 also added in the fuel to reduce the k-eff value. The optimum configuration of UN fuel reached when used heterogeneous core configuration case four with percentage of U-235 in F1=5.5 %, F2=7 % and F3=8.5 % also with the addition of Np-237 0.2 % and fuel fraction 56 %. It has a maximum excess reactivity value 12.56 % $\Delta k/k$. And then, the optimum configuration of ThN fuel reached when used heterogeneous core configuration case three with percentage of U-233 in F1=2 %, F2=4 % and F3=6 % with the addition of Pa-231 0.5 % and fuel fraction 53 %. It has a maximum excess reactivity value 7.67 % $\Delta k/k$. The comparison of optimum design of UN and ThN fuel shows that the ThN fuel has the k-eff value closer to critical than UN fuel. Therefore, in this study, ThN fuel is more suitable for use in PWR reactors because it has a small excess value and can operate for 10 years without refueling

Keywords: PWR, SRAC, thorium nitride, uranium nitride, modular reactor, excess reactivity

COMPARISON OF THORIUM NITRIDE AND URANIUM NITRIDE FUEL ON SMALL MODULAR PRESSURIZED WATER REACTOR IN NEUTRONIC ANALYSIS USING SRAC CODE

Ratna Dewi Syarifah

Corresponding author

Doctor of Physics, Principal Investigator*

E-mail: rdsyarifah.fmipa@unej.ac.id

Mila Hidayatul Aula

Undergraduate Student, Research Assistant*

Andini Ardianingrum

Undergraduate Student, Research Assistant*

Laela Nur Janah

Undergraduate Student, Research Assistant*

Wenny Maulina

Master of Science*

*Department of Physics

Universitas Jember

Jl. Kalimantan Jember, 37, Krajan Timur,
Kecamatan Sumbersari, Kabupaten Jember,
Jawa Timur, Indonesia, 68121

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1. Introduction

In 2020, global electricity demand fell by 1 % because of the Covid-19 pandemic. According to the newest data, global electricity demand is estimated to increase by 4 % in 2022 due to global economic recovery, especially in the Asia Pacific region [1]. The rate of electricity demand is proportional to the rapid growth of electricity generation from renewable energy of 8 % in the last two years. It has an impact on increasing the use of coal power which risks driving carbon dioxide emissions from the electricity sector. Based on this problem, low-carbon technologies, such as nuclear power generation, are becoming the focus of clean energy research [2, 3].

Today, nuclear technology provides about 10 % of the world's electricity with approximately 440 power reactors, and more than 50 countries utilize nuclear energy with 220 research reactors [4]. Based on data, there are 304 PWR-type reactors in operation [5]. PWR (Pressurized Water Reactor)

is one of the first-generation nuclear power plants developed in terms of economy, reliability, and security systems [4].

PWR is a pressurized water reactor that uses light water as a coolant and moderator. PWR has two cooling systems: a primary cooling system and a secondary cooling system. The primary coolant is used to transfer the heat of the fuel to the heat exchanger and forwarded to the secondary cooler. The heat in the secondary cooler will produce steam which is flowed to the generator to generate electricity [6].

PWR nuclear plants that have been commercialized mostly use uranium as their primary fuel. Whereas in nature, especially in Indonesia, thorium resources are more significant than uranium. The neutron output of U-233 in the thermal and epithermal regions is higher than that of Pu-239 in the uranium or plutonium fuel cycle. Therefore, a thorium-based nuclear fuel is proposed to enlarge the fissile. Other reasons identified in previous research were the potential for reduced fuel cycle costs, reduced U-235 enrichment requirements, safer reactor operation due to lower core excess reactivity re-

quirements, and safer and more reliable operation [7]. Therefore, it is necessary developing research on the use of thorium as a PWR fuel and also need to comparing neutronic analysis between thorium and uranium fuels in PWR.

2. Literature review and problem statement

The paper [8] presents the results of research the prospect of uranium nitride (UN) and mixed nitride fuel (UN-PuN) for PWR. Shown, that UN-PuN fuel has a higher *k-eff* value than UN fuel. It means that UN fuel has *k-eff* value approach critical value in reactor, which is means the reactor is stable. But there were unresolved issues related to the comparison of UN fuel and ThN fuel in PWR, because in nature (specially in Indonesia), thorium resources are more significant than uranium. A way to overcome these difficulties by calculating the prospect of thorium fuel in PWR.

This approach was used in [9], research on the use of thorium in PWR reactors for 20–300 MW produced an excess reactivity value of less than 5 % with an operating life of 10 years [9]. Thorium fuel had a higher conversion ratio (CR) than uranium [10]. Neutronic analysis studies of infinite cells show that the addition of Pa-231 is better than Np-237 as a burnable poison in the thorium fuel system. The thorium oxide system with enrichment of 8 % U-233 and 7.6–8 % Pa-231 is the most suitable fuel for PWR cores because it provides less than 1 % excess reactivity and longer burn-up years (up to 20 years) [11]. Research about thorium fuel also has been done [12, 13]. The paper [12] used thorium oxide with SRAC-COREBN with JENDL 3.2/3.3 calculation. For 20 MW reactor, the optimum design able to operate for 10 years with maximum excess reactivity 4.6 % $\Delta k/k$. And the other paper [13] investigated about neutronic design study of small long-live PWR with (Th, U) O₂ fuel. The paper concludes that some property of the thorium-based fuel to the U-233 enrichment and the moderation ratio or fuel fraction [13]. The other research [14] about core design parametric study of integral pressurized water reactor (IPWR) with mixed oxide ceramic fuel using SRAC code system. The period of criticality of reactor core up to 1521 days with lowest CR is 0,622004 [14]. The calculation of 2-Dimensional PWR MOX/UO₂ Core Benchmark OECD NEA 6048 with SRAC Code has been done [15]. Based on the results of these calculations, SRAC code system can be used to generate cross-section and to calculate some neutronic parameters [15].

The comparison of UN and ThN fuel has been done in GFR reactor [16–18]. The paper [16] used (Th, U233) N in fast reactor for 500MW. It has excess reactivity value <2 % and has average power density are 65 Watt/cc. The power density is lower than UN fuel. Other paper [17] present UN and ThN fuel comparison in fast reactor. UN has higher conversion ratio (CR) than ThN fuel. For fast reactor is better use UN fuel than ThN fuel because the needs of breeding ratio in fast reactor. The paper [18] was calculated the neutronic analysis of comparison of UN and ThN fuel in fast reactor (GFR). This research can reach burn up time more than 20 years with excess reactivity less than 1 percent ($\Delta k/k < 1\%$) both UN-PuN and ThN fuel. However, from the paper [8–18], all this suggests that it is advisable to conduct a study on comparing the optimization value of the neutronic calculation between UN and ThN fuel in PWR reactor (thermal reactor).

3. The aim and objectives of the study

The aim of the study is comparing the optimization value of the neutronic calculation between UN and ThN fuel in PWR reactor.

To achieve this aim, the following objectives are accomplished:

- calculating optimization of neutronic calculation of UN fuel for 300MW PWR;
- calculating optimization of neutronic calculation of ThN fuel for 300MW PWR;
- calculating the comparison of neutronics calculation of UN and ThN fuels.

4. Materials and methods

The object of this study is the comparison of UN and ThN fuel on small modular PWR. The UN and ThN fuel have different characteristic material. Both of two fuels could be used in PWR reactor. The hypothesis of this study is ThN has better characteristics material as a fuel in the reactor when viewed from the value of *k-eff* and excess reactivity for thermal reactors such as PWR. This research focuses on the analysis of the neutronic reactor, which calculated by SRAC 2006.

The calculation method uses the SRAC2006 code system with the JENDL 4.0 library as the database. SRAC (Standard Thermal Reactor Analysis Code) is a code system for neutronic analysis for various types of reactors developed by JAEA [19]. The first calculation stage will be done by calculating the fuel pin cells (PIJ) using the JENDL 4.0 data library. The results of the PIJ are the neutron flux, macroscopic, and microscopic data. The data will be used in the second stage, namely the calculation of the reactor core. The calculation of the reactor core is carried out with the code CITATION (Fig. 1). The reactor design configuration uses two types, namely homogeneous and heterogeneous. Homogeneous uses a fuel presentation, while heterogeneous uses various types of fuel presentation. Fig. 1 shows the SRAC Calculation scheme in this research.

SRAC code uses diffusion equation approach. The neutron equilibrium equation contains one group neutron diffusion equation, two groups' neutron diffusion equation, and a multigroup neutron diffusion equation. Multigroup neutron diffusion equation states that the neutrons on the reactor core are distributed in a broad spectrum of energy. Multigroup neutron diffusion equations are obtained by dividing neutron energy into energy groups. Fig. 2 shows the neutron energy group scheme.

Multigroup neutron diffusion equations mathematically can be written as follows.

$$\begin{aligned} \frac{1}{v_g} \frac{\partial}{\partial t} \phi(r,t) = & \nabla \cdot D_g(r) \nabla \cdot \phi_g(r,t) - \sum_{ag} (r) \phi_g(r,t) - \\ & - \sum_{sg} (r) \phi_g(r,t) + \sum_{g'=1}^G \sum_{sgg'} (r) \phi_{g'}(r,t) + \\ & + \chi_g \sum_{g'=1}^G V_{g'} \sum_{fg'} (r) \phi_{g'}(r,t). \end{aligned} \quad (2)$$

The number of neutrons in one group can increase the number affected by several factors, such as neutrons resulting from the reaction to the fission and the neutron scattering [20].

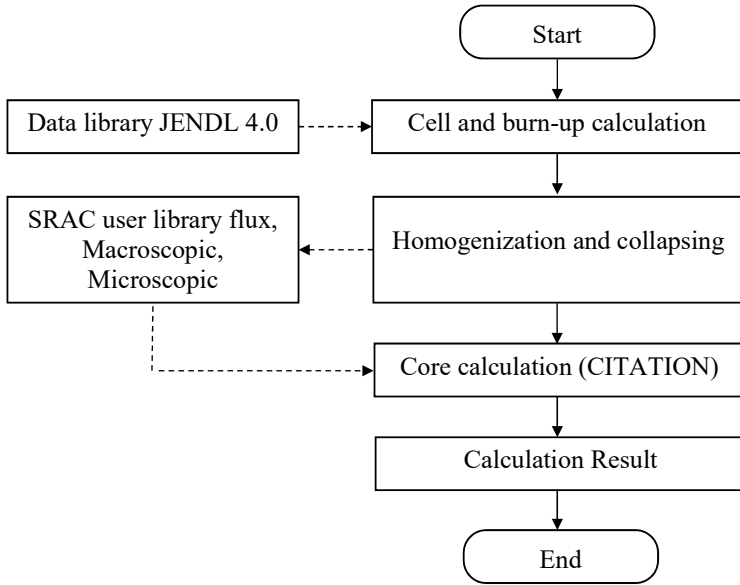


Fig. 1. SRAC Calculation Scheme

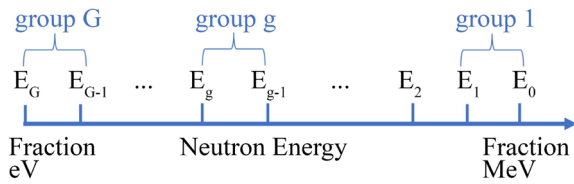


Fig. 2. Neutron energy grouping scheme

This study was conducted to compare two types of fuel in PWR without refueling with an operating time of 10 years. The fuel cell used is in the form of a hexagonal pin consisting of fuel, cladding, and coolant, as shown in Fig. 3. The fuel used is uranium nitride (UN) and thorium nitride (ThN), silicon carbide (SiC) as cladding, and H₂O as a moderator and coolant. The reactor core design uses the pancake cylinder type shown in Fig. 4.

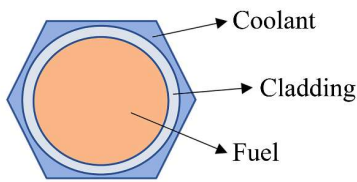


Fig. 3. Fuel cell design with hexagonal pins and its region

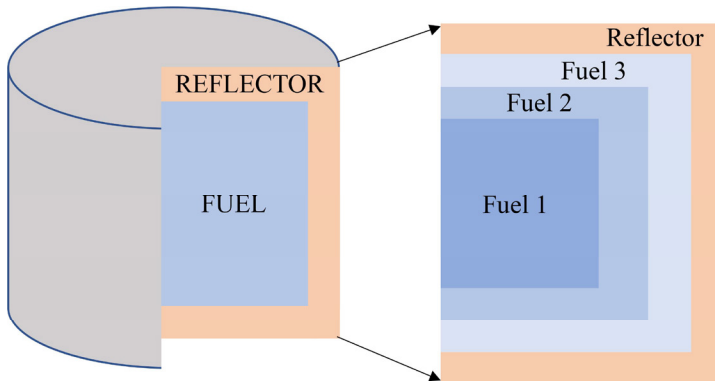


Fig. 4. Reactor core design

Table 1 describes the parameter design of PWR reactor using UN and ThN fuel.

Table 1

Parameter design of reactor using UN and ThN fuel

Parameter	Specification	
Fuel	UN	ThN
Power	300 MW	
Cladding	Silicon carbide	
Coolant	H ₂ O	
Fuel pin design	Hexagonal pin cell	
U-235 fraction	4–14 %	2–10 %
Fuel volume fraction	55–60 %	50–55 %
Cladding volume fraction	10 %	10 %
Coolant volume fraction	35–40 %	30–45 %
The additive in fuel	Np-237	Pa-231
Pin pitch	1.45 cm	
Diameter active core (D)	300 cm	
Height active core (H)	100 cm	
Reflector width	50 cm	

The parameter design consists of fuel pin also fuel core specification. The power was used in this research is 300MW with hexagonal pin cell geometry and cylinder pancake ($D>H$) core geometry. The width of the reflector is 50 cm for each side. The reactor geometry was used in two fuels are the same, but the different one was the detailed specifications of the fuel and additives were included in the fuel.

The comparison of ThN and UN fuel for PWR was used some step was shows in Fig. 5. A neutronic calculation of fuel pin using a PIJ calculation on SRAC for UN and ThN fuel during 10-years burn-up. The research analyses the value of the effective multiplication factor (k_{eff}) based on the homogeneous and heterogeneous core configuration for UN and ThN fuel with CITATION calculation. Fuel optimization was obtained after a neutronic analysis of the fuel, namely homogeneous and heterogeneous core configuration, addition of minor actinide (Np-237 in UN fuel), addition of burnable poison (Pa-231 in ThN fuel), and fuel fraction variations. K_{eff} is the ratio of neutrons produced by fission reaction in one generation to the number of neutrons lost through absorption and leakage in the preceding generation. K_{eff} can be divided into 3 conditions, that is subcritical conditions ($k_{eff}<1$), critical conditions ($k_{eff}=1$) and supercritical conditions ($k_{eff}>1$).

Fig. 5 shows the step of neutronic calculation of comparison UN and ThN fuel. The calculation is divided by three steps. The first step was calculating the optimization of UN fuel with calculating homogeneous core configuration; heterogeneous core configuration; the addition of neptunium-237 (Np-237); and fuel fraction variation. The second step was calculating the optimization of ThN fuel with calculating homogeneous core configuration; heterogeneous core configuration; the addition of protactinium-231 (Pa-231); and fuel fraction variation. The third step was comparison of neutronic calculation of UN and ThN fuels.

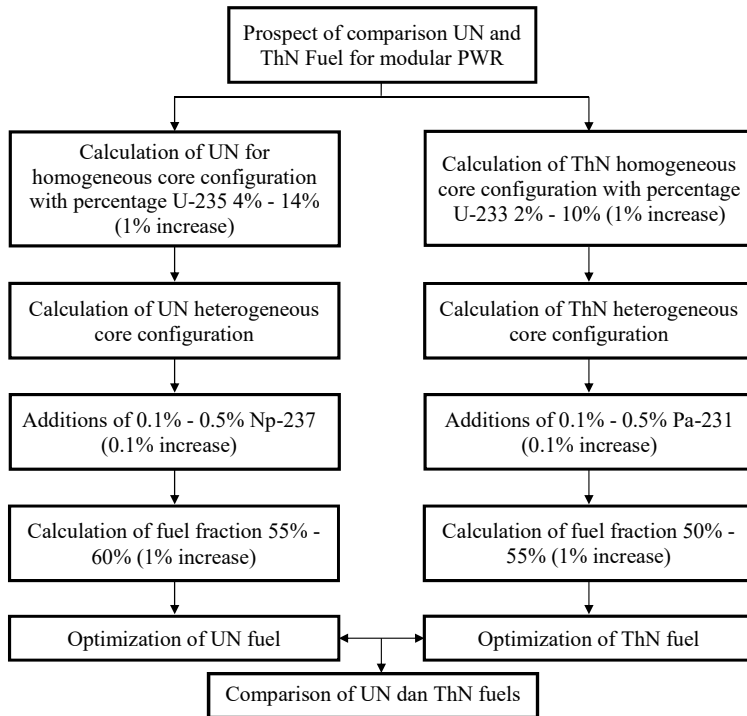


Fig. 5. The scheme of the neutronic calculation of comparison UN and ThN fuel

5. Results of research comparison ThN and UN fuel for pressurized water reactor

5.1. Optimization of neutronic calculation of UN fuel for 300MW pressurized water reactor

Fig. 6 shows the k_{eff} value of UN fuel based on variations in the percentage of uranium 235 (U-235) of 4–14 % using a homogeneous core configuration. Based on Fig. 6, the percentage of U-235 of 7 % has a stable k_{eff} value with a maximum k_{eff} value of 1.1684. So that the percentage of U-235 of 7 % is used as the value to determine the heterogeneous configuration with a combined percentage of three fuels. The maximum value of excess reactivity generated at enrichment 7 % U-235 is 14.42 % $\Delta k/k$. Table 2 show percentage of U-235 variations in heterogeneous configurations for UN fuel.

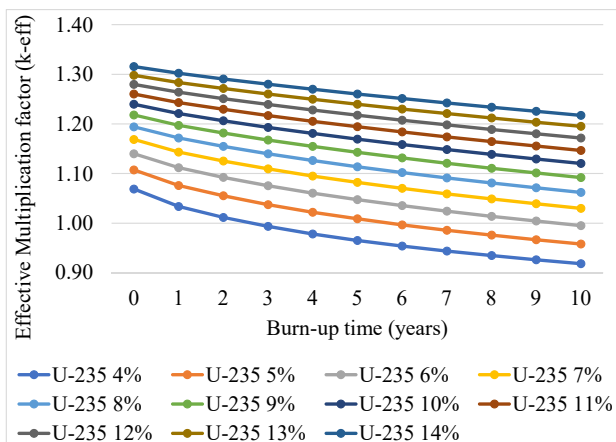


Fig. 6. The k_{eff} value of homogeneous core configuration for UN fuel

Fig. 7 shows the k_{eff} value for a heterogeneous core configuration for UN fuel. The percentage of F2 is constant at

7 %, with the percentage variation on F1 and F3 to calculate five variations (Table 2). Fuels percentages with F1, F2, and F3 of 5.5 %, 7 %, and 8.5 % have the stable k_{eff} value with a maximum k_{eff} value of 1.145048. The maximum value of excess reactivity generated is 12.67 % $\Delta k/k$. A low excess reactivity value generates a low rate of decline in k_{eff} values.

Table 2
Percentage of U-235 variations in heterogeneous configurations for UN fuel

Case	Percentage of U-235		
	F1 (%)	F2 (%)	F3 (%)
1	4	7	10
2	4.5	7	9.5
3	5	7	9
4	5.5	7	8.5
5	6	7	8

Fig. 8 shows the k_{eff} value of UN fuel with the addition of 0.1 % to 0.5 % Np-237. The addition of a larger Np-237 generates a smaller k_{eff} value because Np-237 absorbs neutrons in the reactor. The neutron absorption Np-237 will turn into Pu-239 (a fissile fuel).

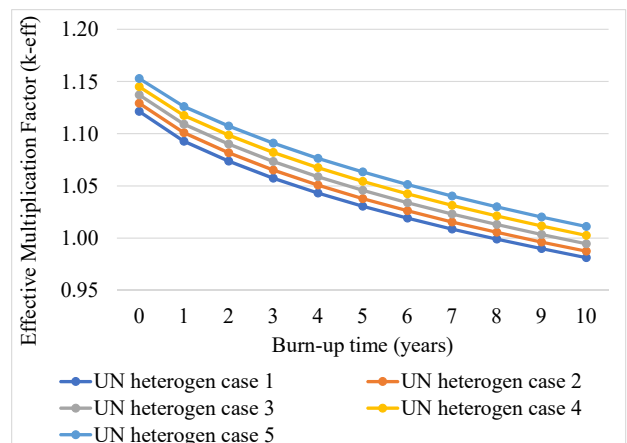


Fig. 7. The k_{eff} value of heterogeneous core configuration for UN fuel

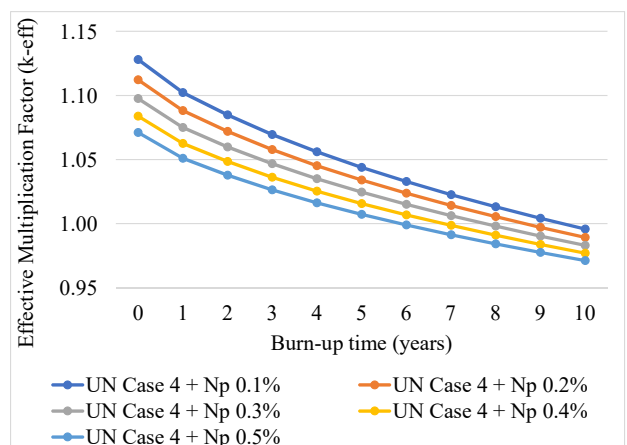


Fig. 8. The k_{eff} value of addition Np-237 in UN fuel

Then, the variation of fuel volume fraction of 55 % to 60 % with an increase of 1 % is shown in Fig. 9. The fuel volume fraction of 56 % has stable k_{eff} with a maximum k_{eff} value of 1.14375, and the value of excess reactivity generated is 12.57 % $\Delta k/k$. Fig. 10 show the optimum k_{eff} value of 300 MW with UN fuel.

The optimum k_{eff} value of UN fuel reached when use heterogeneous core configuration case four with percentage of U-235 in F1=5.5 %, F2=7 % and F3=8.5 % also with the addition of Np-237 0.2 % and fuel fraction 56 % (Fig. 10). The UN fuel optimization has a maximum excess reactivity value 12.56 % $\Delta k/k$.

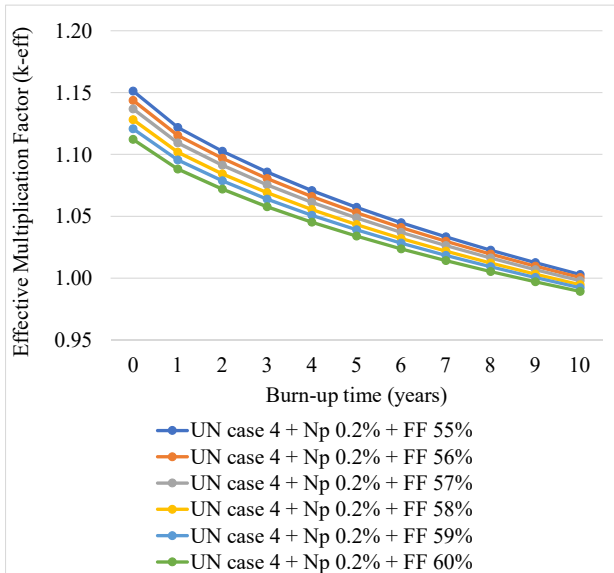


Fig. 9. The k_{eff} value of fuel fraction variations for UN fuel

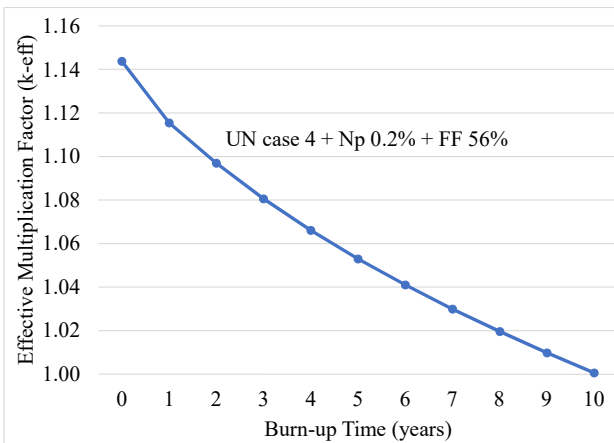


Fig. 10. The optimum k_{eff} value of 300 MW with UN fuel

5.2. Optimization of neutronic calculation of ThN fuel for 300 MW pressurized water reactor

Homogeneous calculations using ThN fuel were performed by the PIJ and CITATION codes to obtain the k_{eff} value. The ThN fuel use U-233 as fissile material. The percentage U-233 is varied from 2 % to 10 %. The graph of the k_{eff} value for homogeneous calculations on ThN fuel is shown in Fig. 11. Based on these results, it is found that the most stable k_{eff} value at the percentage of U-233 4 %.

The next calculation is the calculation of the heterogeneous core configuration with three types of fuel percentag-

es. Fig. 12 shows the k_{eff} value using a heterogeneous core configuration. Based on Fig. 12, shows the fuel in case 3, which was the variation with the most stable k_{eff} value. To reduce the value of excess reactivity, then Pa-231 was added in case three. Pa-231 addition is varied 0.1 % to 0.5 %. Table 3 shows percentage of U-233 variations in heterogeneous configurations for ThN fuel.

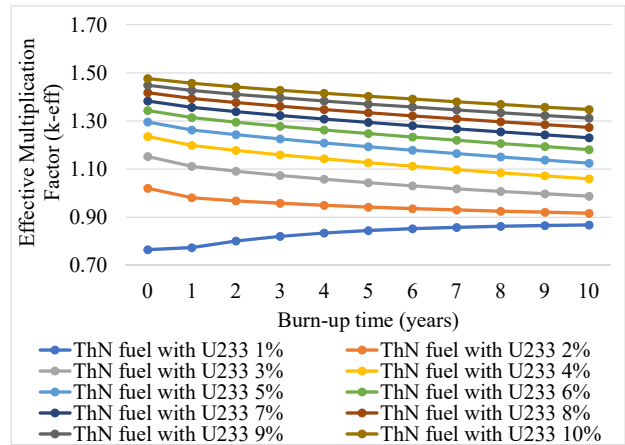


Fig. 11. The k_{eff} value of homogeneous core configuration for ThN fuel

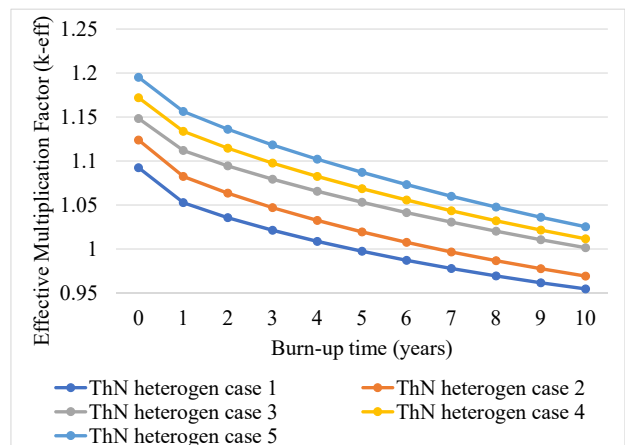


Fig. 12. The k_{eff} value of heterogeneous core configuration for ThN fuel

Table 3

Percentage of U-233 variations in heterogeneous configurations for ThN fuel

Case	Percentage of U-233		
	F1 (%)	F2 (%)	F3 (%)
1	2	3	4
2	2.5	3	3.5
3	2	4	6
4	2.5	4	5.5
5	3	4	5

Fig. 13 shows the k_{eff} value of addition Pa-231 in ThN fuel. The use of the percentage of U-233 in case 3 with a Pa-231 of 0.5 % gives a relatively flat k_{eff} burn-up pattern, as shown in Fig. 13. The k_{eff} value indicates that the reactor conditions are subcritical. Then an analysis of the variation of the volume fraction of the fuel is carried out to optimize the design of the fuel used.

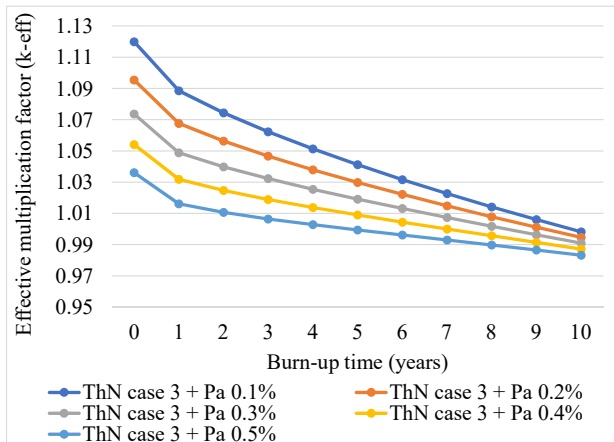


Fig. 13. The *k-eff* value of addition Pa-231 in ThN fuel

Fig. 14 shows the *k-eff* value of fuel fraction variations for ThN fuel. The optimal fuel value is obtained after varying the fuel fraction based on the results (Fig. 14). The most sloping fuel fraction is 53 %, with a maximum *k-eff* value of 1.08309 and a maximum excess reactivity value of 7.67 % $\Delta k/k$. The ThN fuel optimization graph is shown in Fig. 15.

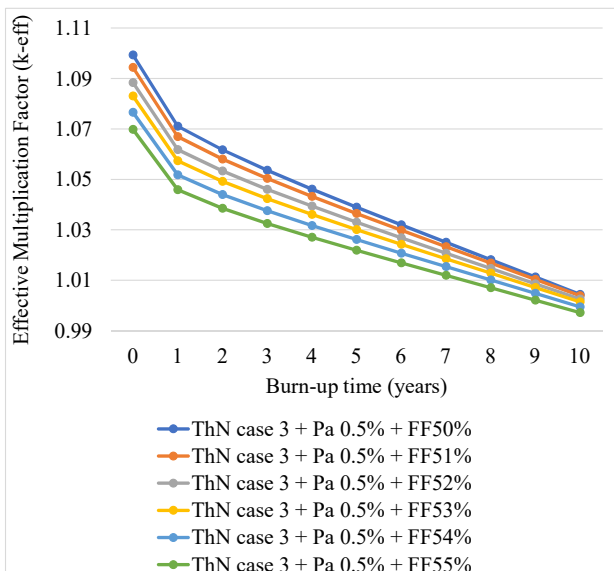


Fig. 14. The *k-eff* value of fuel fraction variations for ThN fuel

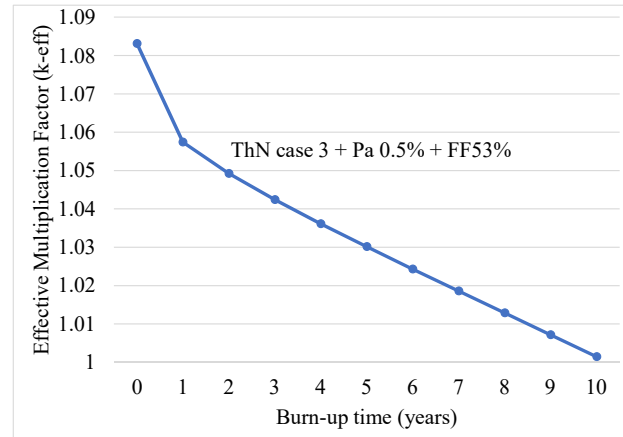


Fig. 15. The optimum *k-eff* value of 300 MW with ThN fuel

The optimum *k-eff* value of ThN fuel reached when use heterogeneous core configuration case four with percentage of U-233 in F1=2 %, F2=4 % and F3=6 % with the addition of Pa-231 0.5 % and fuel fraction 53 % (Fig. 15). The ThN fuel optimization has a maximum excess reactivity value 7.67 % $\Delta k/k$.

5.3. The comparison of neutronic calculation of UN and ThN fuels

Fig. 16 shows the comparison of UN and ThN fuels at optimal conditions. The optimization of ThN fuel reach maximum *k-eff* value of 1.08309 and a maximum excess reactivity value of 7.67 % $\Delta k/k$. And for UN fuel reach maximum *k-eff* value of 1.14375 and a maximum excess reactivity value 12.56 % $\Delta k/k$. According to optimization results and the graph in Fig. 16, ThN has a *k-eff* value more stable than UN. The UN fuel also has excess reactivity greater than ThN fuel. Therefore, ThN with Pa-231 addition is recommended for PWR without refueling with a burn-up time of 10 years.

The comparison of optimum design of UN and ThN fuel shows that the ThN fuel has the *k-eff* value closer to critical than UN fuel. The optimum results obtained on the two fuels are different because each fuel has different characteristics, atomic density values and material properties.

Fig. 17, 18 shows power density distribution at BOL (Beginning of Life) and EOL (End of Life) of optimum *k-eff* value for UN dan ThN fuel.

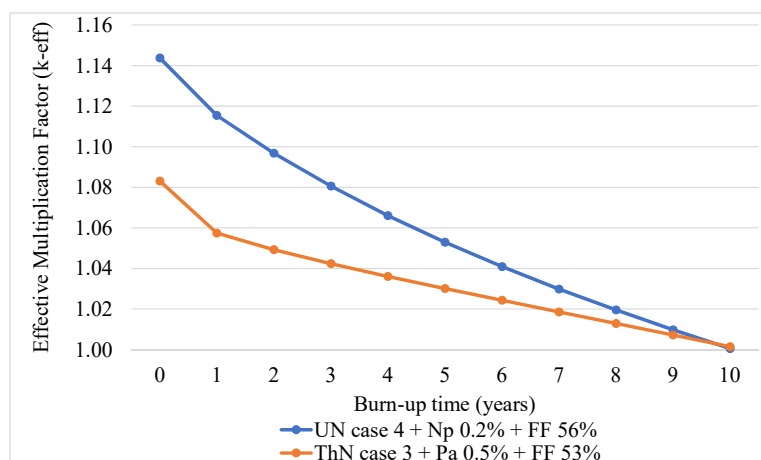


Fig. 16. Comparison of optimum *k-eff* value UN and ThN fuel for 300 MW PWR

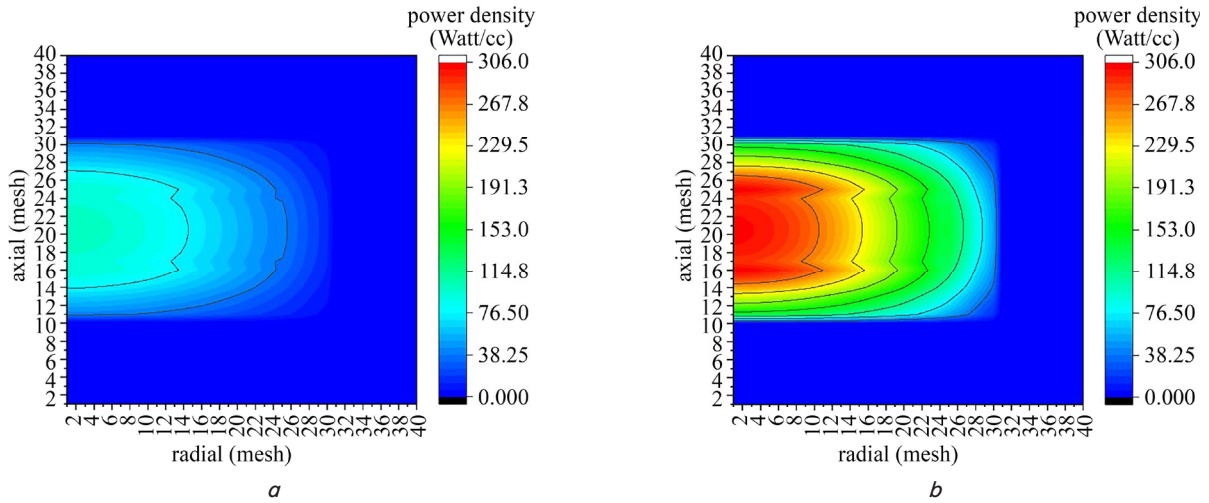


Fig. 17. Power density distribution (Watt/cc): *a* – at BOL (Beginning of Life); *b* – EOL (End of Life) of optimum *k-eff* value for UN fuel

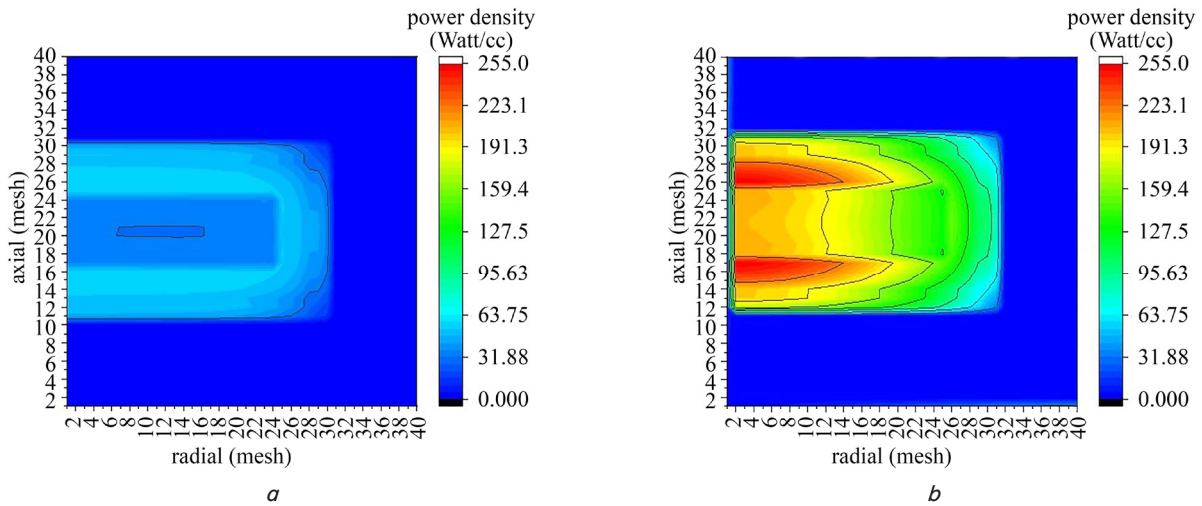


Fig. 18. Power density distribution (Watt/cc): *a* – at BOL (Beginning of Life); *b* – EOL (End of Life) of optimum *k-eff* value for ThN fuel

Fig. 17 show the BOL (in the first year), the power density value around 90 Watt/cc. After ten years (EOL), the power density value increases up to around 300 Watt/cc. The maximum power density value occurs in the center of the core reactor. Fig. 18 show the BOL (in the first year), the power density value around 50 Watt/cc. After ten years (EOL), the power density value increases up to around 230 Watt/cc.

6. Discussion of comparison ThN and UN fuel in neutronics analysis 300 MW

According to the result of UN fuel in Fig. 10, the optimum *k-eff* value of UN fuel reached when use heterogeneous core configuration case four with percentage of U-235 in F1=5.5 %, F2=7 % and F3=8.5 % also with the addition of Np-237 0.2 % and fuel fraction 56 %. The heterogeneous core configuration makes the peaking power density decrease in the central of the core. The addition of Np-237 could decrease the *k-eff* value because Np-237 capture neutron and become Pu-239 as a fissile material (Fig. 9). Therefore, Np-237 could decrease the *k-eff* value in the beginning of burn-up time, and increase it in the end of burn-up time.

According to the result of ThN fuel in Fig. 15, the optimum *k-eff* value reached when use heterogeneous core configuration case four with percentage of U-233 in F1=2 %, F2=4 % and F3=6 % with the addition of Pa-231 0.5 % and fuel fraction 53 %. As same as in the UN fuel, the heterogeneous core configuration could decrease the peaking power in the central of the core. The addition of Pa-231 could decrease the *k-eff* value because it absorbs the neutron to become U-233 as fissile material (Fig. 14).

According to the result of comparison of UN and ThN fuel in Fig. 16, the ThN fuel has *k-eff* value lower than UN fuel. Also, it has *k-eff* value flatter than UN fuel. This is happened because U-233 in ThN fuel has cross section fission greater than U-235 in UN fuel. Therefore, ThN fuel has better fuel prospects than UN fuel in PWR.

These results were obtained using the calculation of the SRAC code, with the same design geometry. The power used in this study is 300 MW which is the power on small modular reactor. This research only calculates the neutronic calculation, so further research is needed to develop the thermal-hydraulic calculation. This needs to be done to determine the safety analysis related to the cooling cycle (flow rate) in the PWR reactor.

7. Conclusions

1. The optimization of UN fuel reached use heterogeneous core configuration case four with percentage of U-235 in F1=5.5 %, F2=7 % and F3=8.5 % also with the addition of Np-237 0.2 % and fuel fraction 56 %. The UN fuel optimization has a maximum excess reactivity value 12.56 % $\Delta k/k$.

2. The optimization of ThN fuel reached use heterogeneous core configuration case four with percentage of U-233 in F1=2 %, F2=4 % and F3=6 % with the addition of Pa-231 0.5 % and fuel fraction 53 %. The ThN fuel optimization has a maximum excess reactivity value 7.67 % $\Delta k/k$.

3. The comparison of optimum design of UN and ThN fuel shows that the ThN fuel has the k_{eff} value closer to critical than UN fuel. The optimum results obtained on the two fuels are different because each fuel has different characteristics,

atomic density values and material properties. The power density distribution at BOL of UN fuel was 90 Watt/cc and ThN fuel was 50 Watt/cc, and EOL of UN fuel was 300 Watt/cc and ThN fuel was 230 Watt/cc. The UN fuel has power density distribution higher than ThN fuel. ThN fuel is more suitable for use in PWR reactors because it has a small excess reactivity value, a stable k_{eff} value and can operate for 10 years without refueling.

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