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Enhancing temperature reactivity coefficients in SMR Reactor with (Th-^{233}U-^{235}U)O_2 fuel through PaO_2 as a burnable absorber

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Abstract

The utilization of (Th-^{233}U)O_2 fuel in thermal reactors, such as in small modular reactors (SMRs), has shown promising potential. However, the less negative to positive moderator temperature feedback coefficient (MTC) stemming from the fission resonances of U-233 at epi-thermal neutron energies remains a concern. Previous studies have proposed incorporating U-235 into the fuel composition, resulting in (Th-^{233}U-^{235}U)O_2, which exhibited improved MTC compared to (Th-^{233}U)O_2 at both beginning-of-cycle (BOC) and end-of-cycle (EOC). However, the MTC values were still less negative than those of traditional UO_2 fuel. This study aims to address the MTC issue by introducing Pa-231 in the form of PaO_2 as an integral burnable absorber (IFBA) coated on the outer surface of the fuel rods. Pa-231, with its capture cross-section of approximately 202 barns at 0.0253 eV, offers significant promise as an absorber and has the potential to act as a fertile material by producing U-233, thus providing an advantage over other absorbers. Simulated results demonstrate that the incorporation of PaO_2 as an IFBA within the fuel considerably adds more negative feedback to the MTC. Moreover, the study reveals that increasing the number of IFBAs within the assembly leads to a more efficient improvement in the MTC. However, it is important to note that this approach results in an increased burnup penalty at EOC due to the presence of residual Pa-231 considering an SMR leakage rate. Further optimization strategies are, therefore, required to mitigate the burnup penalty while maintaining the desired MTC improvements.

Keywords: (Th-^{233}U-^{235}U)O_2 fuel, MTC, IFBAs, PaO_2, SMR.

1. INTRODUCTION

The increasing energy demand from both the industrial and public sectors is heavily dependent on the total population of each country and the growing demands of industries. Governments worldwide are now considering the incorporation of nuclear power plants into their energy mix to meet this enormous electricity demand. SMRs are emerging as a promising solution due to their technological, geographical, and economic advantages [1]. SMRs offer modularity, allowing them to be manufactured and assembled in a controlled manufacturing environment before being transported to the site. This approach reduces on-site preparation and the lengthy construction duration typically associated with larger reactors, resulting in lower construction

costs. Furthermore, the scalability of SMRs makes them particularly suitable for small, isolated areas with low energy demands and limited infrastructure [2][3]. Designing SMRs is a complex task that requires careful consideration of various factors. One crucial aspect is the fuel system, which should have a relatively large internal conversion ratio and improved safety coefficients to ensure continuous and safe operation throughout the burnup cycle [4][5].

Reactivity coefficients, also known as reactivity feedback, are critical in determining a nuclear reactor's inherent safety [6]. They assess how much the core's reactivity changes in response to changes in operating parameters such as fuel depletion, temperature, and absorbers. Temperature changes have a large impact on reactivity, so temperature coefficients of reactivity are critical for reactor safety and control. The fuel temperature coefficient (FTC) and moderator temperature coefficient (MTC) are essential coefficients of the reactivity feedback and should be designed to be negative in order to control the reactor effectively [7]. As a result, calculating and optimizing FTC and MTC are critical aspects of reactor design.

In a previous study, we investigated the neutronic performance of an innovative fuel mixture, (Th-^{233}U-^{235}U)O_2, in an SMR pressurized water reactor (PWR) based on the AP1000 design. The fuel mixture aims to improve the less negative MTC by incorporating U-235 within the (Th-^{233}U)O_2 fuel [8]. Our findings showed that this new fuel exhibited enhanced MTC values compared to (Th-^{233}U)O_2 at both the beginning and end of the burnup cycle. However, the MTC values remained less negative than those of traditional UO_2 fuel due to U-235 depletion and the contribution of regenerated U-233 from Th-232. Therefore, further study is crucial to exploring ways to improve the MTC using (Th-^{233}U-^{235}U)O_2 fuel in SMRs. In this study, our proposal focuses on enhancing the MTC by introducing a neutron absorber called PaO_2. We suggest incorporating PaO_2 as a burnable absorber, which would be coated on the outer surface of the fuel rods [9]. Through the evaluation of multiple cases, we aim to assess the potential improvements in MTC, and FTC, as well as their impact on the criticality period and early reactivity suppression. We provide an overview of PaO2, integral burnable absorber, coated poison technology, and discuss the implemented methodologies in the subsequent sections of the paper.

2. METHODOLOGY AND INPUT PARAMETERS

2.1. Assembly under consideration and code description

Computational codes and data libraries play a crucial role in simulating the behavior of a reactor core and are essential tools for nuclear engineers throughout various phases, including assembly and core design and operation. In this study, the deterministic code DRAGON5 was utilized for calculations [10][11]. Additionally, the evaluated neutron data file library, ENDFB-VIII rel. 0, was used for cross-section data in the evaluation. DRAGON5 is a lattice physics code that solves the neutron transport equation by employing various numerical and estimation methods. The code performs neutron transport computations using 2D and simple 3D geometries and can implement the characteristics method, the discrete ordinates method, or the collision probability. It offers several modules for different functions associated with solving transport or diffusion equations. The modules employed in this study include LIB, GEO, EXCELT, SHI, ASM, FLU, EVO, and EDI [12][13].

For benchmarking purposes, a Westinghouse AP1000 pressurized water reactor (PWR) assembly was selected as the model. Because the AP300 small modular reactor (SMR) with a capacity of 300 MWe (900 MWth) is based on the licensed and operational Gen III+ AP1000 PWR technology, which has demonstrated exceptional reliability in the industry. The fuel assembly consists of a 17 × 17 matrix with 264 fuel rods fueled by standard UO_2 with a maximum enrichment of 4.95 wt.%. Additionally, it incorporates 25 guide tubes (refer to Figure 1). General design data for the considered PWR assembly were obtained from References

[14][15], and the key characteristic parameters are summarized in Table 1. Furthermore, Table 2 provides data for other structural materials used in the assembly.

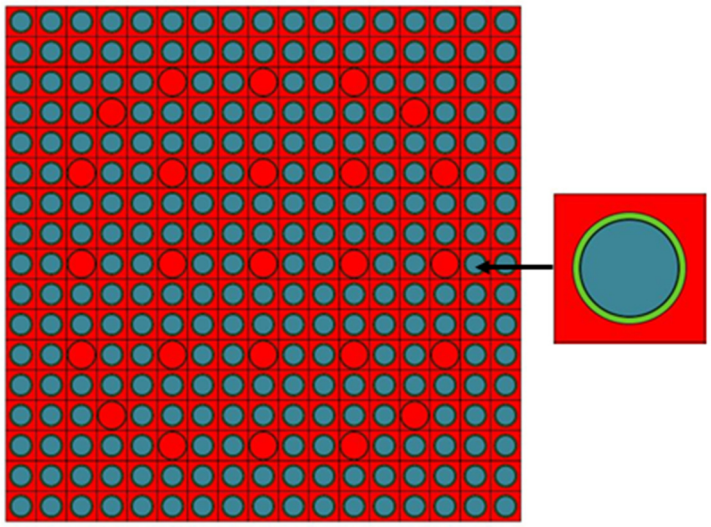


Figure 1. Horizontal layout of PWR fuel assembly by DRAGON code.

Table 1. Geometrical specification of the considered assembly [16].

Parameters	Value
Rod array	17 × 17
Number of fuel rods	264
Number of guide tubes	25
Assembly pitch (cm)	21.5
Rod lattice pitch (cm)	1.260
Fuel outer radius (cm)	0.409575
Helium gap outer radius (cm)	0.417750
Clad outer radius (cm)	0.474750
Guide tube	
Guide tube inner radius (cm)	0.56
Guide tube outer radius (cm)	0.60

Table 2. Data for the examined fuel models and other material specifications [16].

Zone	Parameter	Value
Fuel cladding	Cladding material	Zirlo^{TM}
	Cladding density	6.50 g/cm^3
Gap	Gap material	Helium
	Gap density	1.2049E-02 g/cm^3
Moderator	Moderator material	Light water
	Moderator density at 600 K	0.654 g/cm^3
	Moderator density at 575 K	0.718 g/cm^3
	Soluble boron concentration	0 ppm soluble boron-free
Guide tube cladding	Cladding material	Stainless Steel type 304
	Cladding density	8.03 g/cm^3

2.2. Investigated fuels

This study focuses on the comparison of three different fuel types used in the assembly depicted in Figure 1. All three fuels have the same cumulative enrichment of 4.95 wt %, which corresponds to the maximum low-enriched uranium (LEU) enrichment. The first fuel type utilized is UO_2, which serves as a reference due to its widespread use in nuclear reactors. The second fuel type is (Th-^{233}U)O_2 (Model 1), while the third fuel type is (Th-^{233}U-^{235}U)O_2 (Model 2), which is our proposed fuel based on our previous studies [16][8][13]. Table 3 provides an overview of the properties of the considered fuels, offering a comprehensive comparison between them.

Table 3. Properties of the analyzed fuel type fuel types [8].

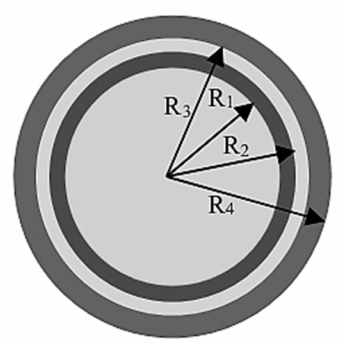
Fuel	Fertile material	Fissile material	Fissile enrichment (wt.%)	Density g/cm^3
UO_2 (Reference)	U-238	U-235	4.95 %	10.53
(Th-^{233}U)O_2 (Model 1)	Th-232	U-233	4.95 %	9.54
(Th-^{233}U-^{235}U)O_2 (Model 2)	Th-232	U-233 & U-235	2.475 % (U-233) + 2.475 % (U-235)	9.54

2.3. Integral burnable absorber

The use of burnable absorbers is a traditional method employed to control neutron generation within an assembly without relying on control rods or other control mechanisms. These absorbers help to reduce reactivity, particularly at BOC [17]. Burnable absorbers can be inserted as discrete rods, coated burnable absorbers, or admixed with the fuel itself, falling into the category known as integral fuel burnable absorbers (IFBAs) [18][19]. In PWR fuel, various IFBAs are utilized, including gadolinium (Gd_2O_3) and erbium (Er_2O_3) [19][20][21]. These materials exhibit significant absorption cross-sections, generate isotopes with small absorption cross-sections through neutron capture, and do not cause physical damage to the fuel or cladding [12]. However, the daughter nuclides resulting from neutron absorption by erbium and gadolinium do not play a significant role in neutronic processes within the reactor core. Therefore, the selection of a burnable neutron absorber whose daughter nuclides positively impact the fission chain reaction is of significant interest. In this study, we propose the use of Pa-231, in the form of PaO_2 coated as a thin layer on the fuel rods (as shown in Figure 2), as a burnable absorber. This choice is advantageous due to Pa-231's moderate capture cross-section of approximately 202 barns, compared to gadolinium (253,254 barns) and erbium (644 barns) [9][22][23]. It is expected that this choice will improve the undesired less negative MTC and also enhance the FTC through increased neutron resonance absorption with rising operating temperatures.

One of the advantages of coated rods is that the absorber is placed on the surface of the rod, avoiding mixing with the fuel and preventing any adverse effects on thermo-mechanical properties. Furthermore, the Pa-231 nuclide offers the potential for reducing early reactivity excess, extending fuel lifetime, and achieving high-level fuel burnup. This is due to its ability to produce U-233 (as presented in Eq. (1), which is advantageous compared to other absorbers. Figure 4 illustrates a cross-sectional view of different arrangements of IFBA rods in the fuel assembly. According to the figure, the IFBA rods are arranged in the fuel assembly with five different configurations, with 28, 44, 72, 88, and 112 IFBA rods [15]. Through the implementation of these IFBA configurations, we aim to investigate their impact on reactivity control, and reactivity coefficients. The detailed analysis and results of the different IFBA rod arrangements will be discussed in the subsequent section, shedding light on the potential benefits and advantages of utilizing PaO_2 as a burnable absorber with (Th-^{233}U-^{235}U)O_2 fuel.

$$^{232}\mathrm{Th} \xrightarrow{(n,2n)} {}^{231}\mathrm{Th} \xrightarrow{\beta^-} {}^{231}\mathrm{Pa} \xrightarrow{(n,\gamma)} {}^{232}\mathrm{Pa} \xrightarrow{\beta^-} {}^{232}\mathrm{U} \xrightarrow{(n,\gamma)} {}^{223}\mathrm{U} \xrightarrow{(n,\gamma)} \ldots \quad (1)$$



Radius	Value (cm)
R1	0.400575
R2	0.409575
R3	0.417750
R4	0.474750

Figure 2. Designed IFBA-coated fuel rod.

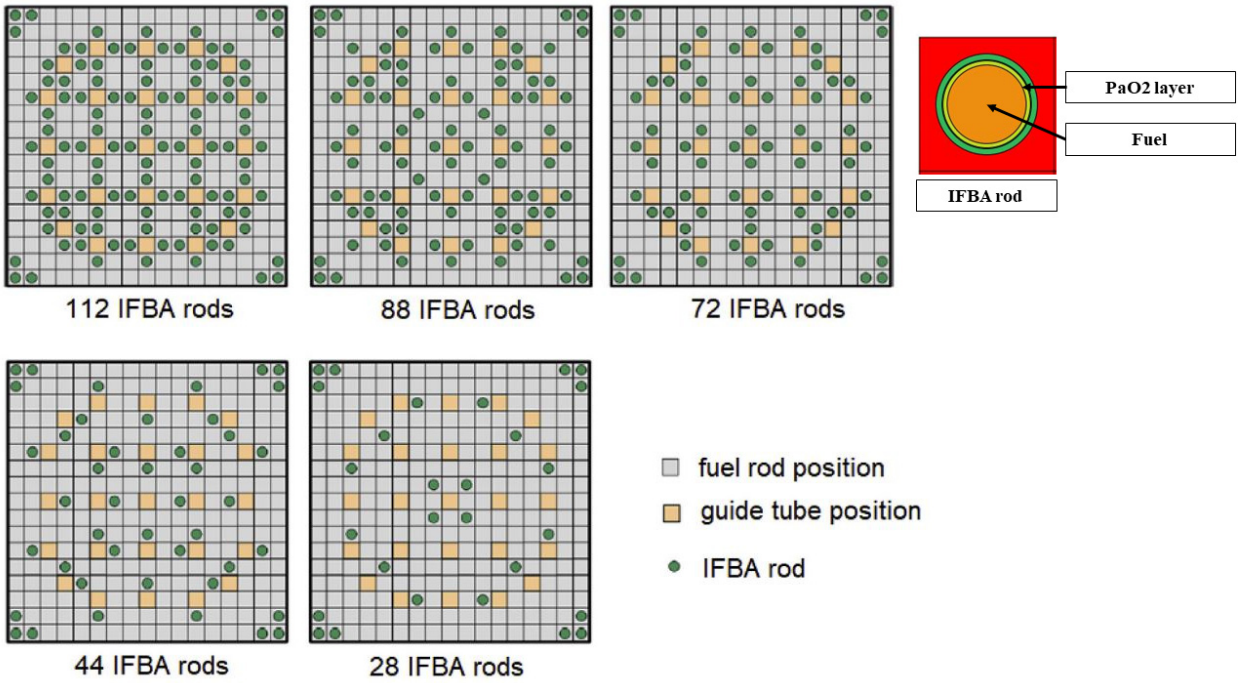


Figure 3. Considered configurations for the IFBA rods in the proposed (Th-^{233}U-^{235}U)O_2 fuel assembly [15].

3. RESULTS AND DISCUSSIONS

3.1. Burnup calculation

The primary goal of this research is to investigate the variations in neutron multiplication factors versus burnup and to determine the criticality periods. The neutron multiplication factor, denoted as K_{INF}, represents the infinite multiplication factor and is calculated assuming the outer surfaces of the fuel assemblies act as reflective surfaces in neutronic calculations. This assumption implies that there is no neutron leakage, and the multiplication factor is exclusively dependent on the properties of the fuel assembly materials. However, the criticality period is strongly influenced by the neutron leakage rate. Neutron leakage has a significant impact on core multiplication, which in turn affects fuel cycle parameters such as burnup and cycle length [24]. Notably, SMRs tend to exhibit higher neutron leakage compared to large power reactors. Typical light water SMRs have been observed to exhibit a neutron leakage rate of approximately 7% [25], while large PWRs have leakage rates of around 3 to 4% [26][27].

In this paper, we consider three different neutron leakage rates: 0%, 4%, and 7%. The 0% leakage case, though impossible to achieve in practice, serves as an ideal reference for comparison. By examining the criticality period with specified neutron leakage rates, our aim is to assess the variations in neutron multiplication factors throughout the fuel burnup cycle. This analysis provides valuable insights into the behavior and performance of different cases, along with their influence on maintaining criticality. Furthermore, understanding criticality periods is crucial for optimizing fuel utilization, ensuring safe and efficient reactor operation, and maximizing fuel lifetime.

Figure 4 illustrates the behavior of K_{INF} as a function of fuel burnup for (Th-^{233}U-^{235}U)O_2 fuel with varying numbers of IFBAs. The results show a two-step decrease in K_{INF} for all cases. The first step corresponds to a rapid decrease caused by the production of Xe-135 and Sm-149, which are significant fission product poisons with thermal absorption cross-sections of 2.65×10^6 barns and 5.85×10^4 barns, respectively. The second step is mainly attributed to fuel depletion. The depletion rate is greatly influenced by the number of IFBAs. As the number of IFBAs increases, the depletion rate decreases. This is primarily due to the slow degradation of Pa-231, which has a relatively small absorption cross-section compared to gadolinium and erbium. Additionally, the transformation process of Pa-231 to U-233 through neutron absorption contributes to the slower depletion rate. In Model 2, as the number of IFBAs in the fuel assembly increases, the K_{INF} value decreases in the early stages of burnup. Because, the incorporation of a neutron absorber in the fuel reduces the thermal utilization factor, resulting in a decrease in K_{INF}. The extent of this decrease is predominantly influenced by the total neutron absorption within the assembly, which, in our case, is determined by the number of IFBAs. Specifically, compared to Model 2 without PaO_2, the K_{INF} at the BOC decreases by 4.64% for 28 IFBAs, 7.44% for 44 IFBAs, 11.86% for 72 IFBAs, 14.14% for 88 IFBAs, and 17.36% for 112 IFBAs.

Figure 5 displays the criticality periods for all the considered models, considering neutron leakage rates of 0%, 4%, and 7%. Among the designs, Model 1 exhibits the highest criticality periods, followed by Model 2 without IFBAs, across all the considered leakage rates. However, both the number of IFBAs and the neutron leakage rates significantly influence the criticality period when a burnable absorber is utilized. Specifically, in Model 2 with IFBAs, the criticality period decreases as the neutron leakage rate increases. This can be attributed to the impact of neutron leakage on the neutron multiplication factor. The balance between neutron production and loss determines the neutron multiplication factor. Neutron loss occurs through absorption (by PaO_2) and leakage from the system. As the leakage rate increases, the criticality period decreases due to a decrease in the neutron multiplication factor caused by greater neutron loss. Moreover, the leakage rate also influences the criticality period of Model 2 with IFBAs compared to the reference case (UO_2). With a 0% leakage rate, all IFBA cases achieve a higher criticality period than the reference. With a 4% leakage rate, only cases with 28 IFBAs, 44 IFBAs, and 72 IFBAs achieve a higher criticality period than the reference. With a 7% leakage rate, only cases with 28 IFBAs and 44 IFBAs achieve a higher criticality period than the reference. These observations highlight the significant influence of both the number of IFBAs and the neutron leakage rate on the criticality period. The results provide valuable insights into the behavior and performance of the different models in an SMR reactor.

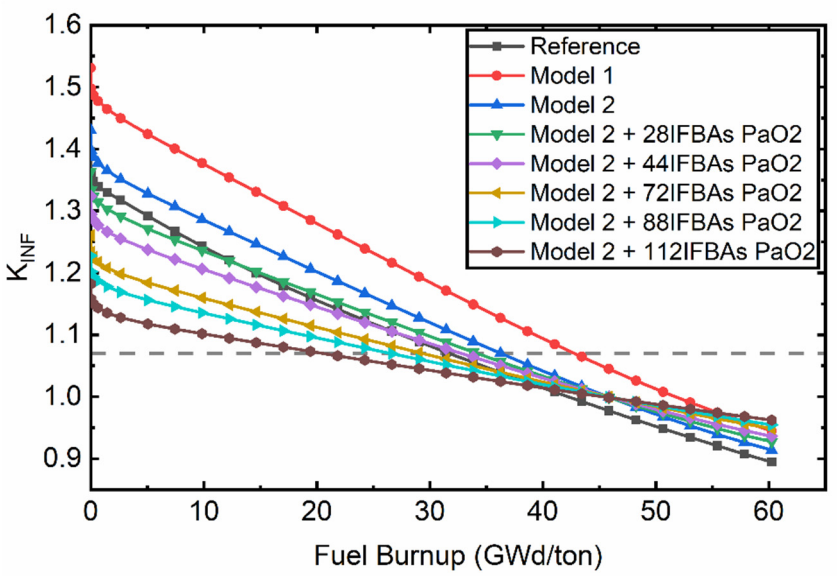


Figure 4. Multiplication factor variation with burnup at different cases of (Th-^{233}U-^{235}U)O_2 fuel with IBFAs compared to Model 1 and the reference.

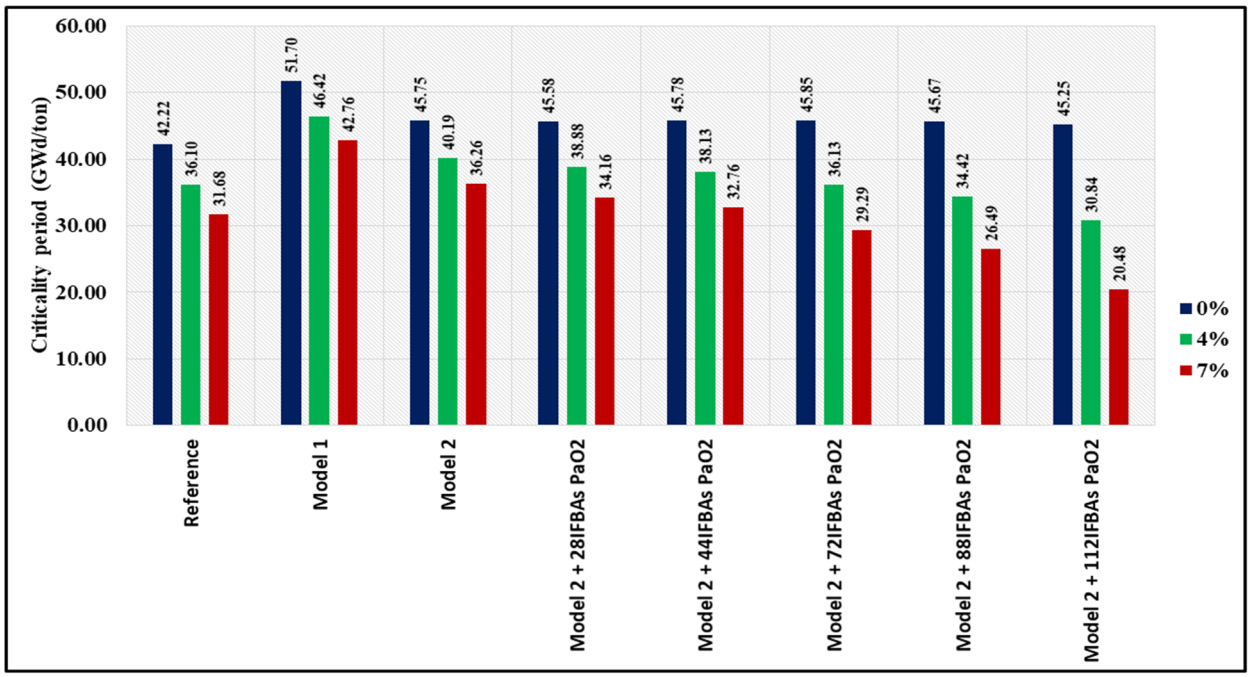


Figure 5. Criticality periods as a function of neutron leakage rates.

3.2. Reactivity coefficients

In this section, we analyze the effects of adding PaO_2 on the reactivity temperature coefficients, specifically the FTC and the MTC. For the calculation of FTC, we consider the moderator and cladding temperatures as constant at 575 K and 600 K, respectively, while varying the fuel temperature from 900 K to 1000 K. In the case of MTC calculation, the moderator temperature is varied from 573 K to 600 K, with the fuel temperature set at 1000 K and the cladding temperature at 600 K. Additionally, the water density is varied from 0.718 g/cm^3 (corresponding to 575 K) to 0.654 g/cm^3 (corresponding to 600 K) for the MTC calculation [28].

Figure 6 presents a comparison of the FTC and MTC evolutions for the different models. The figure demonstrates that the addition of PaO_2 within the assembly introduces more negative

reactivity feedback to Model 2, as observed in both the FTC and MTC, at BOC and EOC. This enhanced negative feedback is attributed to the resonance capture of Pa-231 [9]. Furthermore, increasing the number of IFBAs in Model 2 enhances the resonance absorptions, i.e. increased spatial self-shielding effect, of thermal neutrons accordingly. Because, as the fuel temperature rises, the reactivity variations due to Doppler broadening from Pa-231 captures are amplified [29]. Additionally, the shift of the neutron spectrum to higher energies caused by moderator heating further enhances the Pa-231 capture resonances, thereby slightly mitigating the less negative MTC observed in Model 2. Moreover, the increased number of IFBAs allows the negative reactivity changes caused by Pa-231 captures in the epithermal range to counteract the less negative to positive reactivity effect primarily from U-233 epithermal fission resonances [9]. Additionally, the presence of undepleted Pa-231 near the end of the cycle improves the MTC at EOC. Consequently, a favorable negative MTC and a strong negative FTC can be achieved, ensuring the stability of reactor operation.

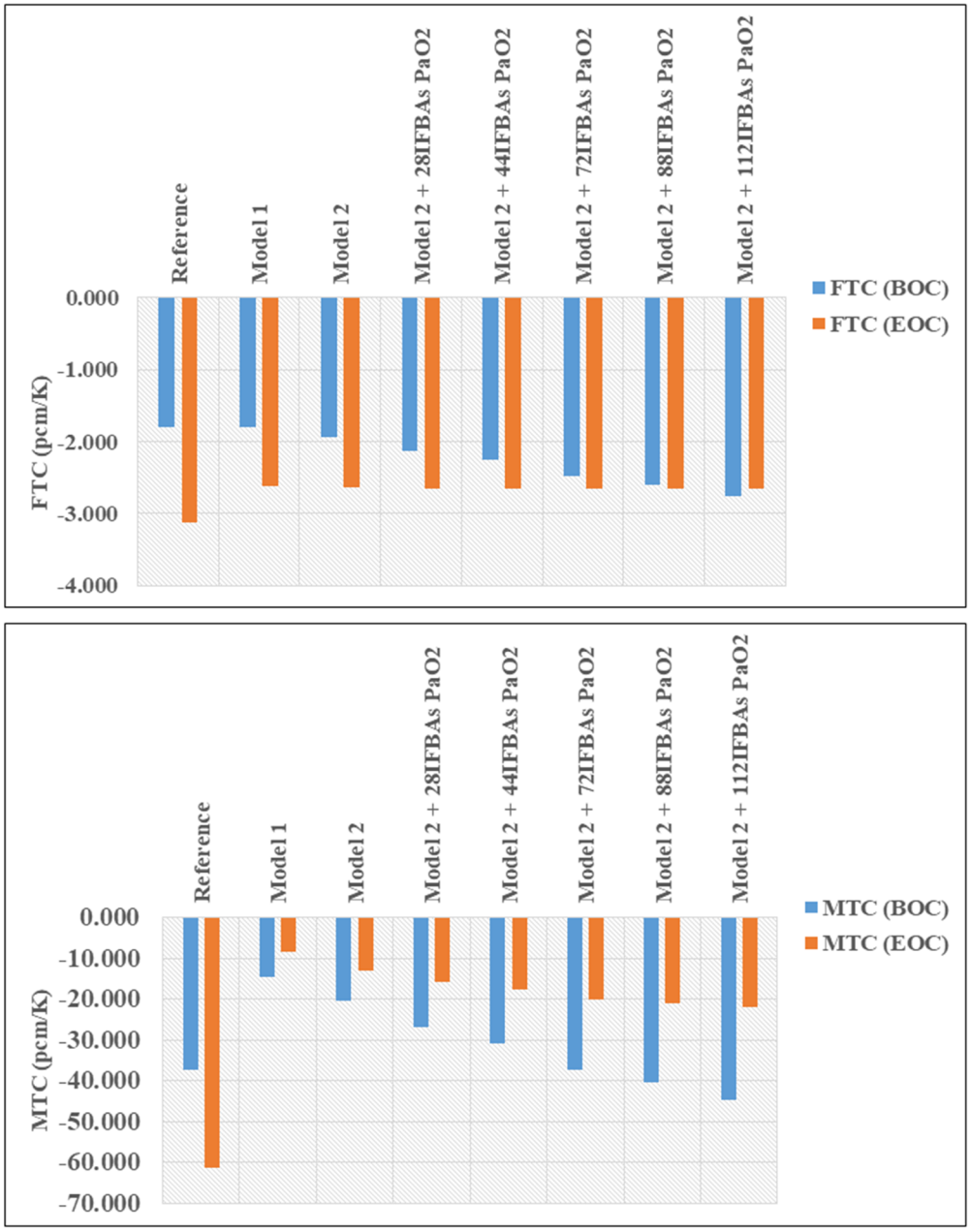


Figure 6. FTC and MTC at BOC and EOC for the different analyzed cases.

4. CONCLUSION

Ensuring a negative MTC is essential for the inherent safety of any reactor. Previous studies have addressed the issue of a less negative to positive MTC for U-233-based fuel by incorporating U-235 into the fuel composition, resulting in (Th-^{233}U-^{235}U)O_2. Although this fuel exhibited improved MTC compared to (Th-^{233}U)O_2, it still had less negative values than conventional UO_2 fuel. In this study, we proposed a solution by adding PaO_2 as a burnable absorber, in the form of integral fuel burnable absorbers (IFBAs), to the (Th-^{233}U-^{235}U)O_2 fuel. The PaO_2 was coated on the outer surfaces of the fuel rods. Our simulations yielded several interesting findings. Firstly, the reactivity at the beginning of the cycle decreased with an increasing number of IFBAs in Model 2 ((Th-^{233}U-^{235}U)O_2), resulting from enhanced thermal absorption within the assembly. Furthermore, the criticality periods were inversely and strongly related to the neutron leakage rate. The analysis of ameliorations on the positive MTC using the proposed solution showed promising results. The strong thermal absorption and resonance absorption in the epithermal regions of Pa-231 contributed to the improvement of the FTC and MTC. Additionally, increasing the number of IFBAs proved to be an effective approach for enhancing both the FTC and MTC.

In summary, (Th-^{233}U-^{235}U)O_2 fuel presents an attractive option for SMRs. The incorporation of Pa-231 as a burnable absorber offers a technically feasible solution to suppress the early excess reactivity and ameliorate the less negative MTC issue caused by U-233. Further research and development in this area can lead to the successful implementation of (Th-^{233}U-^{235}U)O_2 fuel in SMR applications.

Declaration of Competing Interest

The authors declare that they have no known financial or personal conflicts of interest that could have influenced the integrity of the research presented in this paper.

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