



Neutronic Analysis of the AP1000 Fuel Assembly with Accident Tolerant Cladding Materials

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Highlights

- Observation of the change in reactor physics parameters affected by a change in cladding material.
- A deterministic collision probably method was used and compared to MCNP at first.
- Increasing fuel enrichment was needed for fuel assembly using Fe-based cladding material.

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Abstract

An alternative material for fuel cladding was required to prevent oxidation caused by interacting with steam, leading to improvement in core integrity. This study analyzes reactor physics parameters of various cladding material candidates for Pressurized Water Reactor (PWR) such as SS-304 austenitic stainless steel, FeCrAl alloy, APMT alloy, and silicon carbide (SiC) ceramic, as candidate Accident Tolerant Fuel (ATF). The neutronic parameters such as infinite multiplication factor (k_{inf}), and neutron spectrum, while temperature reactivity coefficient related to fuel temperature (DTC) and moderator temperature (MTC) is also considered, followed by a void coefficient of reactivity (VCR) of each candidate material were then compared with ZIRLO as a standard cladding material of AP1000. k_{inf} calculated by SRAC2006 is also compared to MCNP for various fuel assembly types. At the beginning of cycle (BOC), the 2.35% UO_2 using SiC gives a higher k_{inf} than ZIRLO at 937 pcm, while 4.45% UO_2 with 88 IFBA & 9 PYREX at 796 pcm. FeCrAl, APMT, and SS-304 cladding gave a smaller k_{inf} compared to ZIRLO in the range of 11000-14000 pcm at 2.35% UO_2 fuel assembly. The values of DTC, MTC, and VCR were still negative throughout the reactor operation which indicates that the inherent safety feature of alternative cladding was possible for this type of fuel assembly, especially for iron-based cladding material followed by an increase in fuel enrichment.

1. INTRODUCTION

Due to its good neutron economy, zirconium alloy was mainly used in light water reactors (LWR). Zirconium alloy's small neutron absorption gives an advantage as a cladding material, but the increased oxidation rate when interacting with high-temperature steam limits its performance. After the Fukushima Daichi nuclear accident, developing a material to substitute zirconium alloys became a major concern, and various research was conducted for Accident Tolerant Fuel (ATF) [1-4]. These studies explore the use of SiC and other Fe-based metals as cladding material combined with UO_2 or substituted with U_3Si_2 which has better heat transfer properties than UO_2 on the Small Modular Reactor (SMR) or typical large reactor (i.e. APR1400) fuel assembly. Other reactors such as CANDU will need enriched uranium to overcome a lower reactivity affected by the changes in fuel material, the use of Fe-based cladding material, or other ATF concepts. Various cladding material has been studied that has a lower oxidation rate at higher temperatures. For this reason, the new cladding material must be able to provide a similar or better neutron

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economy so it could support efficient energy production at LWR besides reducing the reactor core damage probability in an accident.

The Research Organisation for Nuclear Energy of the National Research and Innovation Agency (ORTN BRIN), the National Energy Agency (BATAN), as a nuclear energy research institute, has carried out various research activities related to the safe operation of LWRs. [5-8]. These studies cover neutronic parameters of PWR benchmark cases such as KOEBERG, IAEA-3D, and BIBLIS that have been carried out using our coupled neutronic and thermal-hydraulic code, NODAL3. Other benchmark cases i.e. PWR rod ejection cases, uncontrolled control rods withdrawal at zero power benchmark of Nuclear Energy Agency-Nuclear Science Committee (NEA-NSC), and NEA-CRP 3D LWR Core Transient Benchmark. Either static or transient cases have been carried out, while sensitivity analysis of node size and time step affecting peak power or temperature evolution such as fuel temperature and coolant temperature have been done.

Studies on the neutronic parameters of the AP1000 as an advanced LWR have been carried out [9,10]. Both studies use standard UO_2 fuel and ZIRLO alloy cladding material and are modeled using MCNP to calculate the kinetic parameters and also modeled using SRAC to generate multigroup cross-sections and derivative constant used on NODAL3 code to determine reactivity coefficient. However, these studies were developed with an oversimplification of their model, so that even with good agreement on the global parameters, such as the effective multiplication factor or the temperature coefficient of reactivity, the radial power distribution and the control rod worth didn't agree well with the design document.

This study was part of the mission to improve our AP1000 core model and focused on testing the consistency/sensitivity of our fuel assembly models by making changes to the material composition to develop an accident-tolerant fuel. In this study, the candidate accident tolerant cladding material being tested was Silicon carbide (SiC), austenitic stainless steel (SS-304), and ferritic iron-chromium-aluminum alloy, either generic (FeCrAl) or its commercial variant (APMT). Other studies on material modification on reactor core components have been done, i.e. AP1000 core that modified to use U-Zr alloy as fuel material that has higher heavy metal density and thermal conductivity, which shows some reduction on safety margin related to the maximum fuel temperature of U-Zr alloy and fuel expansion, so further studies are needed to improve to the safety margin [11]. Other modifications such as coating for the zirconium cladding using chromium and FeCrAl also have been done for the NuScale reactor core, with U_3Si_2 silicide fuel substituting UO_2 to reduce temperature gradient with its higher thermal conductivity while maintaining a promising neutronic performance [12].

SiC cladding has a good performance at high temperatures, good corrosion resistance, and oxidation resistance for up to 1700°C , with lower neutron absorption [13]. The unfavorable properties of SiC as a fuel cladding material are its decrease in thermal conductivity due to defects created by neutron irradiation [14, 15]. However, SiC-based materials show good oxidation resistance and strength in contact with steam at high temperatures making this cladding material a good candidate as an alternative cladding material. FeCrAl cladding which has high oxidation resistance at high temperatures and less hydrogen generation in reactor accidents also has a low corrosion rate but its thermal neutron absorption is quite high in comparison to zirconium cladding [16].

APMT material as advanced FeCrAlMo alloy has good corrosion resistance to water, good oxidation resistance at high temperatures, stable, and has high thermal conductivity [17]. Various studies in optimizing fuel enrichment and fuel rod geometry can minimize the effects of higher neutron absorption so APMT is being considered for alternative cladding materials in nuclear power plants. SS-304 stainless steel as a cladding material is also good at steady and transient reactor operating conditions. The main disadvantage of SS-304 alloy is its high absorption cross-section when compared to zirconium alloy.

The objective of this study was to perform a sensitivity analysis of the SRAC2006 lattice code for a typical fuel assembly based on existing AP1000 design data, followed by an analysis of the neutronic parameters of various alternative cladding materials. The neutronic calculations conducted using the SRAC2006

program were validated with the MCNP by comparing the infinite multiplication factor (k_{∞}) of various AP1000 fuel assemblies. The previous calculation of the PWR neutronic parameters with various Monte Carlo Code shows a good agreement which indicates good modeling consistency on each model, such as a modification of fuel and cladding material on APR1400 using Serpent, reactivity and temperature reactivity coefficients of VVER using MCNP, and modification of AP1000 to introduce mixed oxide fuel using MCNP6 [18-20]. Other neutronic parameters being investigated in this study were k_{∞} , temperature coefficient of reactivity either Doppler for fuel temperature (DTC) or moderator temperature (MTC), and void coefficient of reactivity (VCR), while accumulated plutonium as a function of burnup also considered. Calculated results of SiC, FeCrAl, APMT, and SS-304 cladding material were also compared with ZIRLO as reference material.

2. METHODOLOGY

The neutronic parameters of the AP1000 fuel assembly were carried out using the SRAC2006 program [21]. SRAC2006 has been used to solve neutron transport and its performance has been validated using the IAEA in-core fuel management benchmark and the OECD NEA PWR Mixed Oxide Fuel (MOX/EO₂) transient benchmark with their results in both cases showing a good agreement to reference data [22-24]. The PIJ module of SRAC2006 was used to solve the fuel lattice with CPM (Collision Probability Method) and PEACO as additional resonance treatment. As lattice code, the 2D model with reflective four sides has been applied, while the nuclear data library of The Evaluated Nuclear Data File ENDF/B-VII.0 with 107 neutron energy groups has been used. This paper also performs k_{∞} calculations for various AP1000 fuel assemblies with the SRAC2006 code system and the MCNP to ensure that calculations with SRAC2006 are sufficiently consistent.

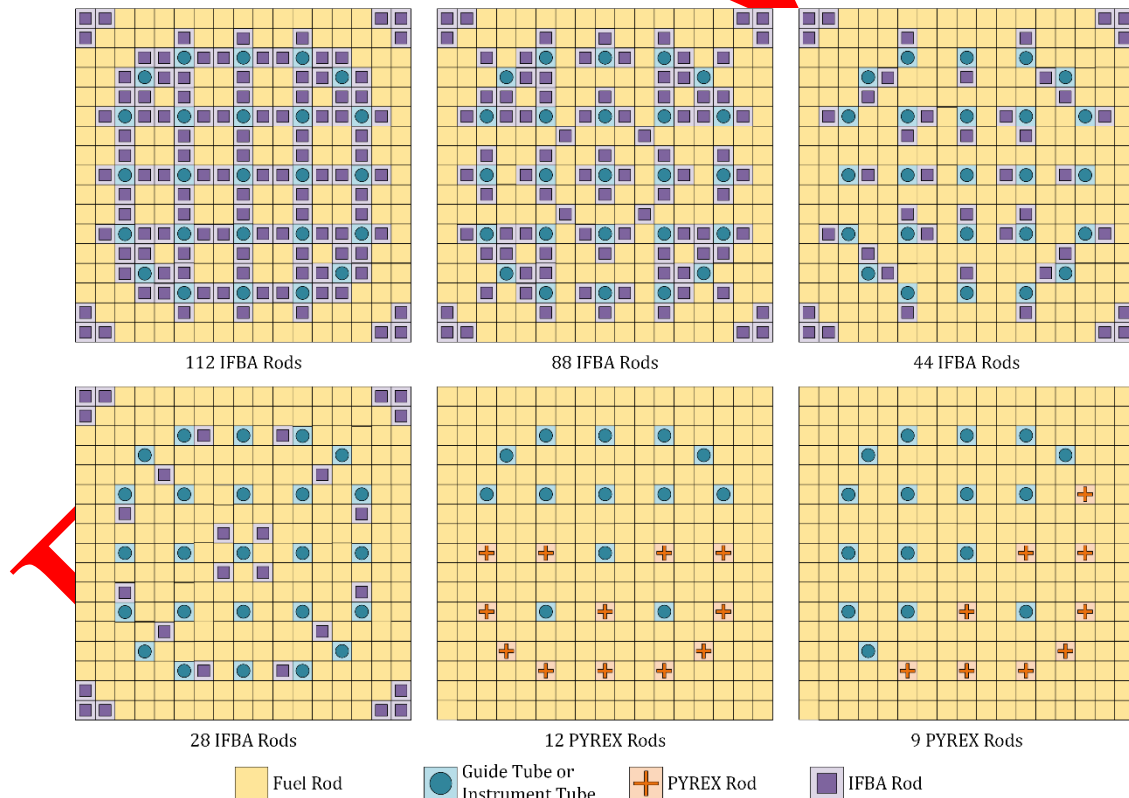


Figure 1. AP1000 fuel assembly types evaluated in this study [25]

AP1000 17×17 fuel assembly with 2.35 % enrichment and ZIRLO cladding material used as reference case that consists of 264 fuel pins, 25 guide tubes, and light water as coolant and neutron moderator as shown in Figure 1, while Table 1 shows fuel assembly parameters [25]. The composition of cladding materials varied shown in Table 2, namely zirconium alloys (ZIRLO) as reference cladding material, SS-304,

FeCrAl, APMT, and SiC. Calculations were made on chosen fuel assembly types on Hot Full Power (HFP) conditions with 900 K of fuel temperature while cladding temperature was set at 557.55 K, and coolant with a boron concentration of 1184 ppm was also set at 557.55K.

Table 1. AP1000 fuel assembly parameters [25]

Parameters	Value
Fuel assembly rod array	17×17
fuel assembly active height, cm	426.7
# fuel rods per assembly	264
# guide tube/instrumentation tube assembly	24+1
Rod pitch (cm)	0.629
Fuel rod outer diameter, cm	0.950
Fuel gap thickness, cm	0.0165
Clad thickness, cm	0.0572
Fuel material	UO ₂ sintered
Fuel density, g/cm ³	10.96(95.5% TD)
Fuel pellet diameter, cm	0.81915
Integral Fuel Burnable Absorbers material	Boride coating
B-10 Content, mg/cm	0.772
Radius of guide tubes inside/outside, cm	1.123/1.224
Coolant density, g/cm ³	0.7194
Boron concentration, ppm	1184

Table 2. The cladding material composition [26,27]

Material (w/t %)	ZIRLO	SS-304	FeCrAl	APMT	SiC
Fe	0.15	71.35	75.00	69.79	-
Cr	0.10	18.90	20.00	21.60	-
Al	-	-	5.000	4.90	-
Zr	98.25	-	-	0.10	-
Ni	-	8.35	-	-	-
Sn	1.50	-	-	-	-
Mn	-	0.70	-	-	-
Mo	-	0.27	-	2.80	-
Y	-	-	-	0.12	-
Si	-	0.43	-	0.53	70.08
Hf	-	-	-	0.16	-
C	-	-	-	-	29.92

3. RESULTS AND DISCUSSION

3.1. Depletion k -Infinity

Preliminary calculations were done to calculate k -inf for the UO₂ fuel element with ZIRLO cladding material using SRAC2006 and MCNP for consistency check, the results were presented in Table 3. From the small relative error of both calculated k -inf, it could be concluded that fuel assembly modeling in SRAC2006 was consistent with the MCNP model for each fuel assembly type. From this point, the calculation was done only with SRAC2006.

Table 3. *k-inf* of various fuel assemblies calculated with SRAC2006 and MCNP

Fuel assembly type	SRAC2006	MCNP	MCNP stdev	%error relative to MCNP
Fuel assembly 2.35%	1.33523	1.33470	0.00007	0.0397%
Fuel assembly 4.45% with 112 IFBA	1.29422	1.29371	0.00009	0.0394%
Fuel assembly 3.4% with 88 IFBA	1.23852	1.23857	0.00008	-0.0040%
Fuel assembly 3.4% with 28 IFBA	1.34892	1.34947	0.00008	-0.0408%
Fuel assembly 3.4% with 44 IFBA	1.31781	1.31812	0.00008	-0.0235%
Fuel assembly 2.35% with 28 IFBA	1.26935	1.26936	0.00008	-0.0008%
Fuel assembly 4.45% with 9 PYREX+88 IFBA	1.26838	1.26884	0.00009	-0.0363%
Fuel assembly 4.45% with 12 PYREX and 88 IFBA	1.24911	1.24874	0.00010	0.0296%

Table 4 presents the calculated *k-inf* of chosen fuel assembly types with cladding material being varied at the Beginning of Cycle (BOC). The 2.35% enrichment of UO_2 fuel assembly at BOC with SiC cladding material gives 0.86% higher *k-inf* than ZIRLO chosen as a reference material in this calculation. Using FeCrAl and APMT material gives a 10% smaller *k-inf*, followed by SS-304 which is 12.6% lower compared to the ZIRLO. Another fuel assembly of 4.45% enrichment with 112 IFBA rods at BOC for SiC cladding gives a similar trend as before, 0.77% higher, while FeCrAl and APMT are around 6% lower and SS-304 was 7.4% lower than ZIRLO. In general, the use of IFBA fuel pins could reduce the neutronic impact of substituting ZIRLO cladding material at BOC with a similar trend also seen on another fuel type of 4.45% enrichment with 112 IFBA and 9 PYREX. The use of SS-304 cladding gives the lowest *k-inf* compared to other cladding materials since nickel (Ni) used in SS-304 has a high absorption cross-section in comparison to aluminum (Al) being used on FeCrAl, leading to a higher neutron absorption rate on SS-304 material.

Table 4. *k-inf* in various fuel assembly and cladding

Fuel assembly type	<i>k-inf</i>				
	ZIRLO	SiC	FeCrAl	APMT	SS-304
UO_2 2.35 %	1.10361	1.11298	0.99132	0.98592	0.96421
UO_2 4.45%, 112 IFBA	1.13314	1.14183	1.06736	1.06602	1.04961
UO_2 4.45%, 88 IFBA, 9 PYREX	1.11187	1.11983	1.04812	1.04690	1.03107

As a basis for reasoning, these studies focus on the neutronic performance of candidate cladding materials, and it could be seen that SiC could provide a good neutron economy as shown by the global parameter of *k-inf*. But, in the case of the safety aspect of an accident-tolerant fuel (ATF), we need to consider various aspects such as its stability during normal operations and transients, while also focusing on the main goal of reducing hydrogen generation since cladding material will contact to high-temperature steam. SiC's superiority over other materials in its *k-inf* gives an advantage in the neutronic aspect but the decrease in thermal conductivity after being irradiated could give some challenges to SiC consistency during operation, either ceramic or composite material. Steel-based material is still considered in this study to show its performance as a material candidate for ATF while also presenting some challenges of sustaining the neutronic aspect.

To simplify this paper, as the trend is repeated in other fuel assembly types, the only fuel assembly type to be discussed is the UO_2 fuel assembly with 2.35% enrichment, without IFBA and PYREX. Reactivity changes of 2.35% UO_2 fuel assembly with various cladding materials are shown in Figure 2, followed by its difference to ZIRLO as reference cladding material.

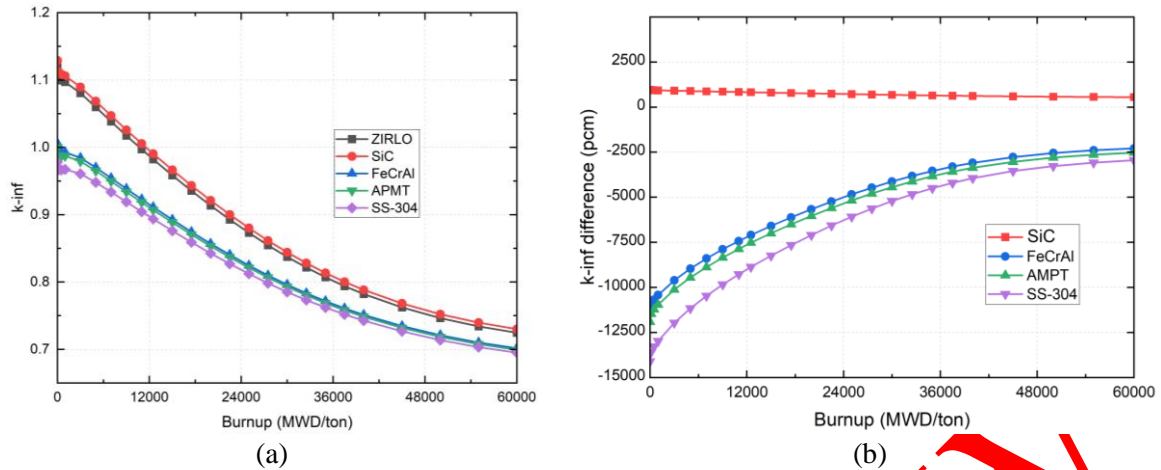


Figure 2. k_{inf} (a) and the difference (b) of other cladding material k_{inf} from ZIRLO cladding versus burnup for fuel UO_2 (2.35 %), boron 1184 ppm

As shown in Figure 2, the k_{inf} values for all cladding materials decrease throughout the fuel burnup and this decrease was caused by lower fissile material even though there is an increase in plutonium produced within the fuel assembly, it was not enough to sustain a nuclear chain reaction, but the neutron spectrum shifted to become hardened, as shown in Figure 3. At the End of Cycle (EOC), 60,000 MWd/ton, The SiC cladding that could absorb fewer neutrons gives higher a k_{inf} of 0.76 % in EOC. The k_{inf} reduction on SS-304 reached almost 4.07% lower than ZIRLO. While the FeCrAl and APMT alloys were slightly lower by 3.16% and 3.49%, respectively. Even FeCrAl has a higher iron content than SS-304, but FeCrAl does not have nickel which has a stronger neutron absorption than aluminum. To increase reactivity to sustain core cycle length, it is mandatory to modify the geometry of the fuel assembly or if necessary, to increase the enrichment of fissile materials within the fuel pellet.

Figure 3 presents a normalized neutron flux per lethargy at the beginning of the cycle of each cladding material, with a relative difference to ZIRLO cladding material also shown. As shown in Figure 3, ZIRLO and SiC cladding materials which have less neutron absorption cross-section than other cladding materials tend to have a high thermal neutron spectrum that is good for a thermal reactor neutron economy. Alternative cladding materials with relatively high neutron absorption tend to have a lower thermal spectrum and higher fast-to-epithermal neutron or neutron spectrum hardening.

The FeCrAl, APMT, and SS-304 reached 15% lower than ZIRLO on thermal neutron flux (peaked at 0.123 eV) as shown in Figure 3, which makes the epithermal and fast neutron fraction increase by up to 5%. It could be seen from the peak of the fast neutron spectrum at energy 0.821 to 1 MeV for SS-304, APMT, and FeCrAl cladding is higher than ZIRLO and SiC. Above this high-energy neutron, it could be seen that ZIRLO and SiC were making some comeback with their higher neutron spectrum which came from a higher fission rate caused by the thermal neutron. These phenomena relate to fission neutron spectrum shifting effects by neutrons inducing fission at first.

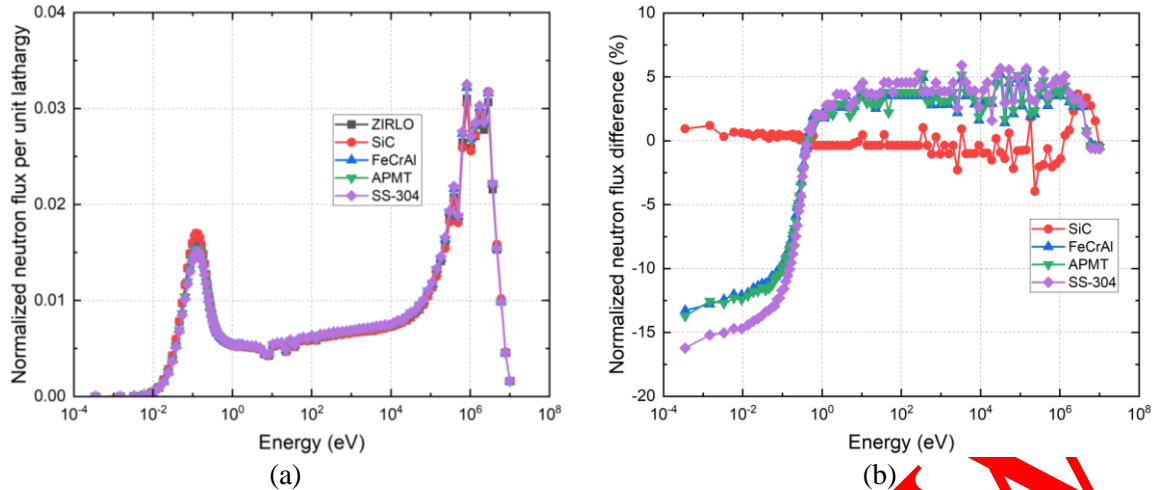


Figure 3. Neutron flux spectrum (a) for various cladding material at BOC and its difference to ZIRLO reference cladding material (b)

Figure 4 presents the accumulation of Pu-239 and U-235 (atomic density) during the fuel assembly burnup for the candidate cladding materials. The density of Pu-239 being produced was increased with some tendency to follow an order of cladding material that has a harder neutron spectrum. Fe-based cladding material with high thermal neutron absorption tends to consume less fissile material at high burnup, resulting in higher Pu-239 and U-235. A harder neutron spectrum could also lead to a higher neutron capture rate of U-238 in the epithermal and resonance regions, increasing plutonium production. Even though more fissile material exists within the fuel assembly, it could not support the reactivity since thermal neutron absorption of Fe-based cladding material results in lower k_{inf} of SS-304, APMT, and FeCrAl compared to ZIRLO and SiC at EOC.

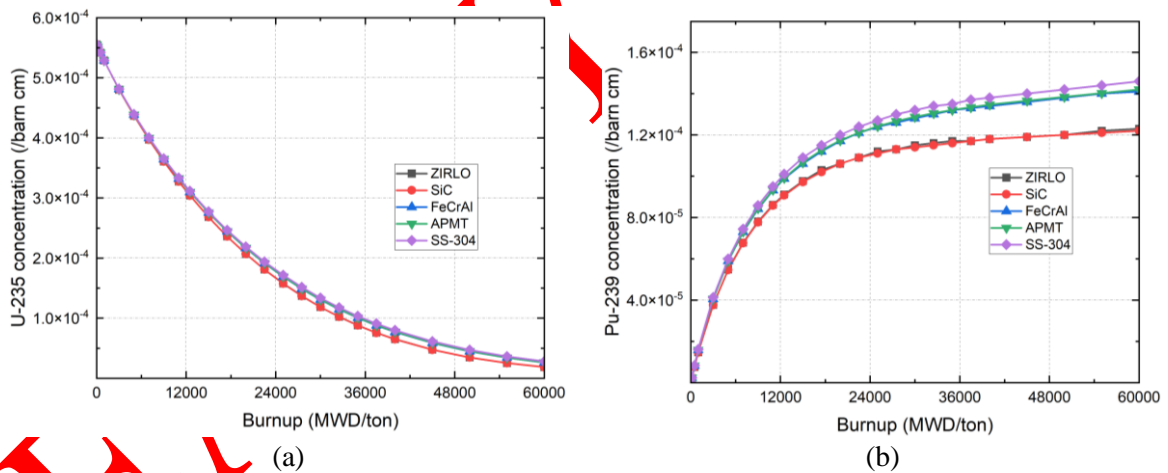


Figure 4. Concentration of U-235 (a) and Pu-239 (b) for various cladding materials

3.2. Doppler Temperature Coefficients (DTC)

DTC was defined as the change in reactivity for a fuel temperature change, so it is one of the most important reactivity coefficients related to the safety of PWR operation with each candidate cladding material must have a negative DTC, especially in the early period of fuel burnup when fuel has high reactivity. The DTC is determined under HFP conditions, with moderator and cladding temperatures set at 557.55 K, while the fuel temperature is changed from its average operating temperature of 900 K to 1200 K. The DTC for different cladding materials is shown in Figure 5, which shows a negative value over the fuel lifetime for alternative cladding materials. The DTC is more negative through the end of the cycle since its fissile material has decreased compared to BOC and results in a higher capture-to-fissile ratio since more fertile material i.e. U-238 affects fuel assembly reactivity. SS-304 cladding exhibits a slightly more negative DTC value compared to other claddings due to the Doppler broadening on fertile material. Figure 5 also shows

the differences in the DTCs of the various cladding materials in comparison to ZIRLO (reference cladding material) while Table 5 shows the DTC values at the BOC and EOC with the DTC values varying from -1.909 to -3.609 pcm/K.

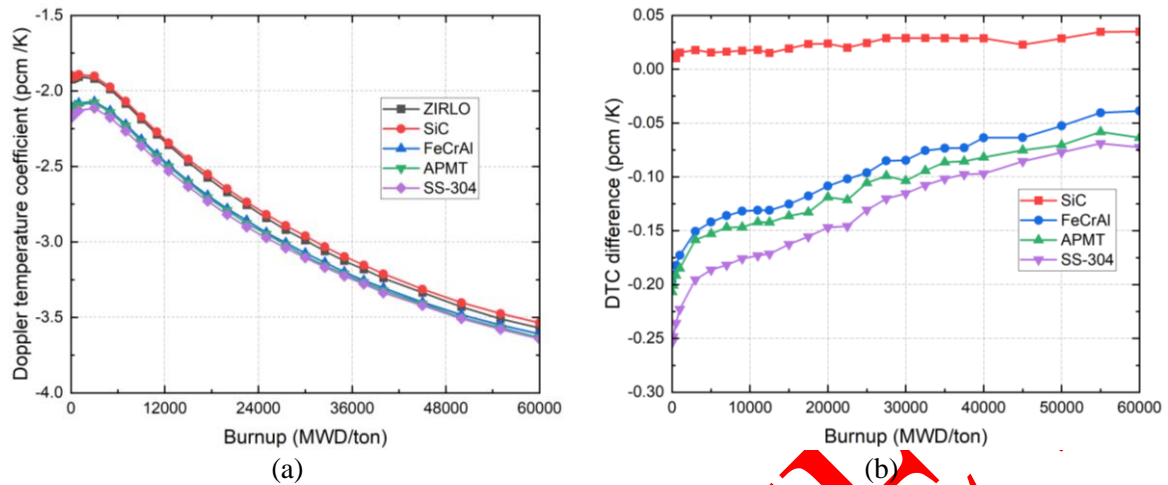


Figure 5. Doppler temperature coefficient of reactivity (a) and the difference of other cladding material DTC from ZIRLO cladding (b) versus fuel burnup

Table 5. DTC of different fuel-cladding materials (pcm/K)

Cladding type	ZIRLO	SiC	FeCrAl	APMT	SS-304
BOC (0 MWD/ton)	-1.9090	-1.8951	-2.1067	-2.1160	-2.1590
EOC (60000 MWD/ton)	-3.5710	-3.5360	-3.6090	-3.6340	-3.6430

3.3. Moderator Temperature Coefficient (MTC)

Since PWR uses light water as a neutron moderator and coolant, when it comes to the change of moderator temperature, its density will change, resulting in a change of neutron moderation, affecting the neutron spectrum. MTC is focused on the changes in moderator temperature only and it is evaluated as part of safety parameters for reactivity feedback during reactor operation. In the MTC calculation, the water temperature was changed from 557.55 K to 598 K. The results of the MTC calculation are shown in Figure 6, which has a negative value throughout the fuel lifetime for all cladding materials. MTC values for SS-340, APMT, and FeCrAl cladding are more negative than ZIRLO and SiC.

Figure 6 shows the MTC value difference from ZIRLO cladding material while Table 6 summarizes the MTC value on BOC and EOC for each cladding material. As shown in Table 6, the MTC value varied from -34,824 pcm/K to -91,461 pcm/K, which corresponds to the negative reactivity feedback throughout the fuel assembly lifetime. The difference in MTC for the alternative cladding is due to the difference in resonance capture on coolant, which affects the overall capture-to-fission ratio when coolant temperature increases.

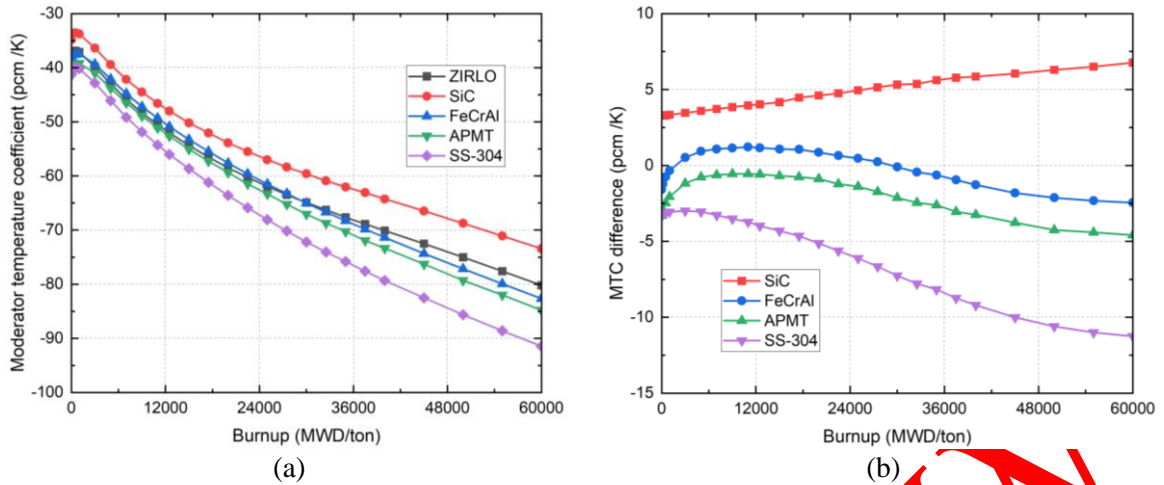


Figure 6. Moderator temperature coefficient of reactivity (a) and the difference of other cladding material MTC from ZIRLO cladding (b) versus fuel burnup

Table 6. MTC of different fuel-cladding materials (pcm/K)

Cladding type	ZIRLO	SiC	FeCrAl	APMT	SS-304
BOC (0 MWD/ton)	-38.113	-34.824	-39.697	-41.421	-41.285
EOC (60000 MWD/ton)	-80.203	-73.436	-82.653	-84.787	-91.461

3.4. Void Coefficient of Reactivity (VCR)

VCR was determined by a change in reactivity caused by the void fraction which changes coolant or moderator density. The void coefficient of reactivity was important for design optimization because it relates to reactivity changes in the reactor core when an accident occurs, especially ones followed by coolant boiling. So, having a more negative void coefficient of reactivity for nuclear safety will be better. VCR was calculated by reducing the moderator density from 0% - 5% due to void fraction, with 0% voids based on a nominal moderator density of 0.7194 g/cm^3 , and the temperature was kept at 576.55 K. Negative VCR could be seen on various cladding material as shown in Figure 7, followed by its relative difference to ZIRLO cladding. Table 7 summarizes the VCR curve on BOC and EOC, and the VCR for ZIRLO cladding at EOC is more negative than the other claddings. The values for VCR are negative from -347 to -837 pcm/% void, and it is shown that the fuel-to-moderator ratio affects VCR in contrast to MTC which is rooted in the moderator temperature, but all negative values ensure the reactor safety.

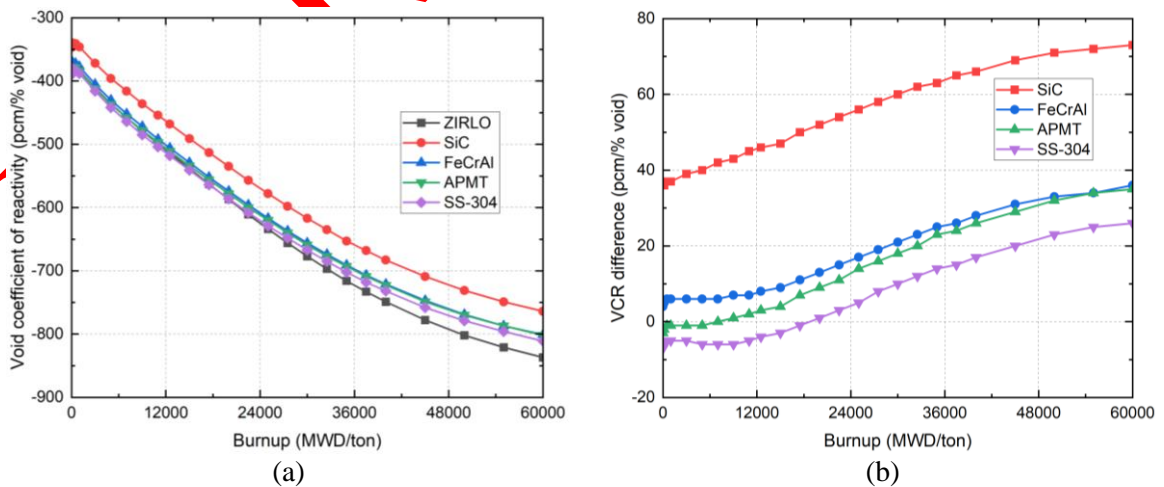


Figure 7. Void coefficient of reactivity (a) and the difference of other cladding material VCR from ZIRLO cladding (b) versus fuel burnup

Table 7. Void coefficient of reactivity of different fuel-cladding materials (pcm/% void)

Cladding type	ZIRLO	SiC	FeCrAl	APMT	SS-304
BOC (0 MWD/ton)	-383	-347	-379	-386	-390
EOC (60000 MWD/ton)	-837	-764	-801	-802	-811

4. CONCLUSION

Neutronic calculations have been carried out for the AP1000 PWR fuel assembly using reference cladding material ZIRLO, and candidate for alternative cladding material such as SiC, FeCrAl, APMT, and SS-304. The calculation results show that the cladding material has an impact on various safety parameters. SiC shows a higher k_{inf} than ZIRLO, FeCrAl, APMT, and SS-304 claddings which are rooted by the thermal neutron absorption rate of SiC that was smaller than other cladding materials. At the BOC of FeCrAl, APMT, and SS-310 cladding shows more negative DTC and MTC than SiC or ZIRLO cladding materials. Spectrum hardening in a fuel cladding with iron-based cladding material such as FeCrAl, APMT, and SS-304 leads to an increase in plutonium accumulation. A similar trend also generally occurs in other fuel assemblies that use IFBA fuel pin and PYREX burnable absorber pin i.e., UO_2 4.45% fuel enrichment and 112 IFBA compared to ones that have 9 PYREX within it, but with lower change in the neutronic parameter in comparison to fuel assembly without IFBA and PYREX. Increasing the core reactivity can be done by increasing the enrichment of uranium or geometry optimization, especially the heat transfer performance, and post-irradiation examination, followed by an economic analysis of applying this alternative cladding concept.

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Note: Calculations done in this study were performed using SRAC2006: A Comprehensive Neutronics Calculation Code System by the Reactor Physics Group of Nuclear Science and Engineering Directorate of Japan Atomic Energy Agency. The license of this Code System has been obtained by Surian Pinem.

CONFLICT OF INTEREST

No conflict of interest was declared by the authors.

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