



Neutronic design of a PWR fuel assembly with accident tolerant-composite for the long-life core

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Highlights

Neutronic investigation of the composite fuels including UN- 30 wt. % U_3Si_2 and 33 vol. % UO_2 -UN for a long-life core in a PWR has been conducted in comparison with that of the conventional UO_2 fuel.

For implementation of the accident tolerant fuel concept, the conventional Zircaloy-4 cladding is replaced with SiC cladding material.

It is possible to achieve sufficient criticality up to 100 GWd/tHM burnup without compromising the safety parameters.

Abstract: For the future of nuclear power, the design and development of an economical, accident tolerant fuel (ATF) for use in the current pressurized water reactors (PWRs) are highly desirable and essential. It is reported that the composite fuels are advantageous over the conventional UO_2 fuel due to their higher thermal conductivities and higher uranium densities. Due to higher uranium densities of the composite fuels, the use of composite fuels would lead to the significant increase of discharged burnup, thereby enhancing fuel cycle economy compared to that of the UO_2 fuel. The higher thermal conductivities of composite fuels will increase the fuel safety margins. For implementation of the accident tolerant fuel concept, this study also investigates on the replacement of the conventional Zircaloy-4 cladding with SiC to minimize the hydrogen production due to interaction of water with cladding at high temperature. In the present work, neutronic investigation of the composite fuels for a PWR has been conducted in comparison with that of the conventional UO_2 fuel. Numerical calculations have been performed based on a lattice model using the SRAC2006 system code and JENDL-4.0 data library. Various parameters have been surveyed for designing a fuel with the UO_2 and composite fuels such as U-235 enrichment, fuel pin pitch. In order to reduce the excess reactivity, Erbium was selected as a burnable poison due to its good depletion performance. The temperature coefficients including fuel, coolant temperature reactivity coefficients, and both the small and large void reactivity coefficients are also investigated. It was found that it is possible to achieve sufficient criticality up to 100 GWd/t burnup without compromising the safety parameters including that four reactivity coefficients are considered those associated with the fuel temperature, coolant temperature, small (5%) void and large (90%) void. Further analysis of the performance of the UO_2 and composite fuels in a full core model of a PWR is being conducted.

Keywords: UO_2 fuel, composite fuels, PWR assembly, neutronic analysis.

1. INTRODUCTION

1.1. Motivation for consideration of alternate fuel and cladding concepts

Nearly all nuclear fuel made with uranium dioxide (UO_2) pellets and zirconium-based cladding has been successfully used for all power reactors, [1], [2], [3], [4]. The

conventional fuel, UO_2 , is stable, and has a high melting point $2850\text{ }^\circ\text{C}$, [5]. However, the UO_2 has a rather low thermal conductivity, $7\text{ W/m}\cdot\text{K}$ at 573 K [5], which decreases with increased temperature and burnup, leading to significant temperature gradients within the ceramic pellets, and would result in thermal stress and potential cracking, [6]. The zirconium alloys, having very low neutron capture cross-section, are used in reactor design to support and contain the fuel pellets, as well as containing fission products. On the other hand, zirconium is vulnerable to oxidation in steam at elevated temperatures. Once an energetic exothermic, hydrogen producing reaction is occurred, it would lead to early cladding failure.

The accidents at Fukushima Daiichi in March 2011 and the Three Mile Island accident in 1979 showed that the current fuel was not adequate and sufficient for the beyond design basis accidents. These beyond design basis accidents would occur at somewhat higher frequencies than previously predicted, and that the financial liabilities of such accidents can cripple a utility [7]. Following the Fukushima Daiichi nuclear accident in 2011, the world nuclear fuel R&D activities have shifted to pursue new fuel materials that provide significant increases in the time for the reactor operator to respond to unforeseen events before significant releases of the fuel materials and fission products occur [8], [9]. The accident tolerant fuel (ATF) systems have attracted significant attention to mitigate the consequences of a future severe accident, by better retaining fission products and/or providing operators more time to implement emergency measures of commercial light water reactors. The desired ATF needs to against a loss of cooling for a considerably long period, and improve fuel performance while enhancing fuel safety at normal operation. Any developed ATF

products would increase operating cost, and enhance safety for commercial application. It is described in the previous studies, [10], [11], the development of ATF/cladding systems are focused on:

(1) Improve or replace the ceramic oxide fuel: aims are to increase uranium loading; to increase thermal conductivity; and to extend fuel cycles due to higher energy content of fuel without higher enrichment cost.

(2) Modify or replace the zircaloy cladding: goals are to achieve improved oxidation resistance, including application of coating layer; to increase fuel rod failure temperature, resistance to thermal cycling and irradiation induced degradation; to decrease thermal neutron cross section for cladding; to increase resistance to expansion and warping; to increase thermal conductivity; and to reduce rate of oxidation.

According to the previous investigations, [11], [12], the silicon carbide fiber-reinforced SiC matrix ceramic composites (SiC/SiC) is a potential cladding material due to their low thermal neutron absorption cross section, retention of strength up to very high temperatures, good radiation resistance, and good oxidation resistance in air and steam up to temperatures of at least $1600\text{ }^\circ\text{C}$. The study in [13] shows that because of a low neutron absorption, the SiC cladding material could meet lifetime requirements even with a 0.1% reduction in enrichment. Regarding the nuclear fuel, high density fuels including uranium-molybdenum fuels, uranium nitride fuels, uranium carbide fuels, and uranium silicide fuels are being considered for ATF solutions. Uranium mononitride (UN) fuel forms have a long historical application for power reactors [13]. Due to have high uranium loading and high thermal conductivity, the uranium mononitride

is desirably used as a nuclear fuel [14], [15]. However, the reactivity of UN with water has been a concern in nuclear reactor applications [14], [15]. For this reason, uranium sesquisilicide (U_3Si_2) and UO_2 have been combined with the UN as composite fuels to provide a protective barrier. It is reported in previous study, [5], that a fuel composed of UN and U_3Si_2 will significantly improve the fuel's thermal conductivity over UO_2 and increase uranium density and therefore enhancing fuel loading. The studies, [14], [16], also show that the UO_2 -UN composite fuels are advantageous over the conventional UO_2 fuel due to its higher thermal conductivity and higher uranium density. In particular, the UO_2 -UN composite fuel with 33 vol. % of UO_2 has a higher uranium density about 13% and a higher thermal conductivity about 100% at 800°C compared to the UO_2 fuel.

The classic approach to generate nuclear energy is to use fuel made with the uranium dioxide (UO_2) pellets and zirconium-based cladding. This method is successfully implemented on industrial scale level for power reactors. Usually, the fuel concept enrichment requires uranium with U-235 fraction less than 20 % (low enriched uranium, LEU). This low enriched uranium fuel is not treated as a nuclear material for direct use in weapon manufacturing, therefore it gives an upper limitation for challenging the uranium fuels for the long-life core. The approach adopted for this study is to use conventional fuel, UO_2 , and composite fuels, (including UN- 30 wt. % U_3Si_2 [5] and 33 vol. % UO_2 -UN [16]), combining with SiC cladding material to estimate the attainable burnup for a wide range of combinations of lattice pitch, P (referred to as "geometries") of interest and for a number of different uranium enrichments for the long-life core with once-through burning.

1.2. Study objective

The primary objective of the present study is to estimate the attainable burnup, 100 GWd/tHM burnup without compromising the safety parameters, for a wide range of combinations of lattice pitch, P, of interest and for a number of different uranium enrichments. The fuel cell is made with UO_2 , composite fuels, (including UN- 30 wt. % U_3Si_2 referred to as UNSi and 33 vol. % UO_2 -UN referred to as UNO), and SiC cladding. The attainable burnup is the maximum burnup of the fuel discharged from a once-through burning fuel subjected to negative reactivity coefficients during the fuel life. Four reactivity coefficients are considered those associated with the fuel temperature, coolant temperature, small (5%) void and large (90%) void. An infinite multiplication factor (k_{inf}) value at the end of cycle (EOC) is conservatively assumed to be 1.05 for the lattice investigations.

1.3. Study scope

Two types of composite fuels are considered - UNSi and UNO. As far as it is known, these composite fuels have been fabricated, even though laboratory experience exists. The material properties of these composite fuels have been extensively studied and are summarized in some companion papers, [5], [14], [16]. It is shown that these composite fuels tested and found suitable for reactor operation.

The first part of the current study is devoted to a scoping study of PWR unit cell that investigated a wide range of combinations of lattice pitch (P - hereby referred to as "geometries"), and different uranium enrichments of different fuel types including UO_2 , UNSi, and UNO. The aim of this investigation is to determine the neutronicly attainable burnup for each of the geometries and

the different fuel compositions, subjected to negative reactivity coefficient constraints. The reactivity coefficient constraints are all negative for coolant temperature coefficient of reactivity (CTC), prompt fuel temperature coefficient of reactivity (FTC), and the reactivity effect of both small voiding 5 % (SVRC) and large voiding 90 % (LVRC) of the coolant. For the examinations with high U-235 enrichment fuel, it would lead to an initial high reactivity excess. It opens a necessary application of burnable poisons (BP) to reduce initial high reactivity excess as in previous studies [17], [18], [19], [20], [21]. Among these mentioned researches, it is found that selected Erbium as a most promising candidate for the long-life core with once-through burning fuel. Thus, in this study, the excess reactivity is compensated by adding burnable poisons of Erbium.

The second part of the study is devoted to a scoping study of UO_2 , UNSi , and UNO fueled PWR assembly. A detailed neutronic analysis of the maximum burnup fuel offering a minimum uranium enrichments and no expanding beyond the present day fuel cycle technology that the fuel is burnt up to 100 GWd/t [22] is presented.

2. METHODOLOGY

2.1. Analysis tools and calculational model

The calculations for this study were performed with the SRAC code system [23] applied to the lattices configuration using the PIJ module derived 16 energy group libraries generated using the JENDL-4.0 [24]. In this paper, neutronic study investigation is limited to infinite pin cell and assembly level calculation with material, temperature, and fuel cell characteristics listed in Table I and Fig. 1.

The reference geometry and specific power assumed for fuel cells are given in Table

I. The data for the reference unit cell correspond to the Westinghouse PWR fuel design that loaded fuel of the 4.45 % wt. U-235 enrichment, [25]. The typical Westinghouse PWR fuel assembly (FA) of 17x17 array, comprises of 289 total lattice locations, of which 24 are for control rod and 1 in the center is instrument thimble, [25]. In simplified fuel assembly calculational models, no water reflector is modeled and spacer grid effects are neglected as well. As described in the previous section, in order to enhance strength and ductility accident tolerant fuel cladding mitigate against severe, SiC is selected as the cladding material [26]. For the high burnup, i.e., long-life core, especially with a burnable poison of Erbium, it is reasonably expected a hardener neutron spectrum and higher pressure of gaseous fission products compared to the reference case. Thus, for the high burnup, up to 100 GWd/t, the fuel would experience in a condition of high porosity. In this study, the porosity of the fuel is conservatively chosen of 15 %.

2.2. Calculated characteristics parameters

In this study, the investigations are U-235 enrichment with ranging from 5 to 20 % and lattice pitch-to-diameter ratio (P/D) ranging from 1.05 to 2.65. Calculations for each of the cases studied are the achievable once-through burnup and the reactivity coefficients along the fuel life without soluble boron in the water. The achievable burnup is assumed basing on combining of negative reactivity coefficients and infinite multiplication factor (k_{inf}) value at the end of cycle (EOC) is 1.05. For the fuel assembly model, there is no water reflector is modeled and spacer grid effects are neglected as well. The reflective boundary conditions of FA is chosen.

The analysis of each fuel model is included the calculation of the achievable

burnup and of reactivity coefficients of a once-through burning fuel. The reactivity coefficients examined are including the fuel temperature coefficient of reactivity (FTC), the coolant temperature coefficient of reactivity (CTC), and the small and large void coefficients of reactivity (SVRC and LVRC). The FTC is evaluated by increasing the fuel temperature by 100 K - from 950 to 1050 K. For the CTC the water temperature is increased from the nominal value of 576.50 K by 10 K to 586.50 K. In case of void coefficients, both small and large, the temperature of the water is left unchanged while the density of the moderator is reduced by, respectively, 5 % or 90 %.

3. PARAMETRIC STUDY RESULTS

3.1. Single fuel cell analysis

The parametric study is undertaken to estimate the effect of P/D on the attainable discharge burnup. The attainable discharge burnup is assumed to be subjected to negative reactivity coefficient constraints and k_{inf} value at the EOC is 1.05. The pin pitch is considered as a design variable. The soluble boron in the coolant, water, is not accounted for in this study. The burnable poison, Erbium, is doped into the fuel helps to reduce the high excess reactivity.

Table II summarizes the selected characteristics calculation for fuel pin cells with various different initial fuel compositions having different P/D values. Increasing the U-235 enrichment results in increasing of both maximum achievable burnup and k_{inf} value at the BOC as given in Table II and Fig. 2. Higher U-235 enrichment in fuel gives larger P/D ranging to achieve the high burnup. This is because of the increase of fissile isotope, U-235, in the heavy metal inventory. It is found that the fuel of ≥ 15 % wt. U-235 enrichment is potential

for a long-life core design. In order to enhance economy of fuel usage and minimize the high excess initial activities, the fuel of 15 % wt. U-235 enrichment is selected for the UO₂, UNO fuel types, and 17.5 % wt. U-235 enrichment is chosen for the UNSi fuel composition. The required P/D ranging is from 1.25 to 1.85, 1.25 to 1.95, and 1.15 to 2.05 for fuel cell with, respectively, 15 % wt. U-235 of UO₂, 15 % wt. U-235 of UNO, and 17.5 % wt. U-235 of UNSi. The potential maximum achievable burnup would reach up to 120 GWd/t as shown in Table II.

As mentioned in the previous section, the main idea behind the present paper is to use low enrichment uranium as a once-through burning and no expanding beyond the present day fuel cycle technology that the fuel is burnt up to 100 GWd/t. Therefore, the P/D = 1.27, belonged to the required P/D ranges, is preferably chosen option in following investigations. As mention above, the high initial reactivity excess is expected to be suppressed by adding burnable poison of Erbium. In this study, the BP is assumed to be homogeneously mixed to the fuel.

For the identified fuel pin cells (that of 15 % wt. U-235 of UO₂, 15 % wt. U-235 of UNO, and 17.5 % wt. U-235 of UNSi, and P/D = 1.27), Fig. 3, Fig. 4, and Fig. 5 depict the design space of the fuel pin cells loaded different fuel types with BP addition. The possible designs are colored in blue that fulfill all criteria including reactivity safety parameters, moderator temperature coefficient, void coefficients, and Doppler coefficient along fuel cycle. It is found that, with the fuel of ≤ 1.5 % BP addition, even though the fuel cells are fulfilled all safety criteria, the k_{inf} values at some beginning burnup stages are higher than that of the reference fuel cell, k_{inf} being equal to 1.3950 as seen in Table II. For the fuel of \geq

3.5 % BP addition, it is not preferable for designing because of positive feedback reactivity coefficients for both the UO_2 and UNO fuel type. Meanwhile the fuel of ≥ 2.5 % BP addition to the fuel of UNSi is unreasonable for the designing.

Figure 6, Fig. 7 show k -inf evolution as a function of burning time and the BOC neutron spectrum, respectively, for some outstanding cases examined. In this study, the neutron lethargy is defined as $\ln(E_0/E)$, where E_0 is emitted neutron energy, and E is slowing down neutron energy. It is clear to see that the neutron spectra of the preferable design fuel cells are all harder than that of the reference fuel cell. The higher percentage of BP addition in fuel pellet is, the harder neutron spectrum of the fuel cell is, as shown in Fig. 7. This is because of the BP material strongly absorbs thermal neutrons [17], [18], [19], [20], [20]. It is found that that the neutron spectra of the preferable design fuel cells are all harder than that of the reference fuel cell at both the begin of cycle (MOC), and the end of cycle (EOC) as well.

3.2. Fuel assembly analysis

Depletion analysis of the fuel assemblies made with composite fuels and SiC clad is carried out against standard operating conditions and other parameters of the typical Westinghouse PWR fuel assembly. The burnup analysis fuel assembly is carried-out up to 120 GWd/t. The identified fuel pin cells (that of 15 % wt. U-235 of UO_2 , 15 % wt. U-235 of UNO, and 17.5 % wt. U-235 of UNSi, and $P/D = 1.27$), achieved as results in the previous section are used for fuel assembly investigation. The initial k -inf value of the reference fuel assembly, 1.4205, is chosen as the upper value of initial criticality to be controlled for other fuel designs.

The analysis results are summarized in Table 3. The gray colored numbers indicate the companion designs that those k -inf values are higher than controlled value of 1.4205 or feedback reactivity coefficients are positive. It is clear to see that it is possible to use the UO_2 , and composite fuels in long-life core with once-through burning fuel, up to 100 GWd/t burnup without compromising the safety parameters. The required BP addition to fuel is 1.5 to 2.5 % for both UO_2 and UNSi fuel type. Regarding the UNO fuel type, the required BP addition to fuel is 1.5 % for the once-through burning fuel with the target burnup of 100 GWd/t.

The pin-power peaking factor (PPF) of all the proper fuel assembly designs are less than 1.10 at the begin of cycle (BOC), and are all higher than that of the reference assembly (1.068). Figure 8, Fig. 9 show k -inf evolution as a function of burning time and the BOC neutron spectrum, respectively, of the proper fuel assembly designs. The maximum k -inf over cycle of the new designs are comparable to that of the reference assembly at ceiling enrichment of 4.45 wt. % U-235 of UO_2 fuel. This ensures that it is possible control core reactivity once loading the new fuel assembly design into the conventional core. The neutron spectrums of the new fuel assembly designs are all harder than that of the reference fuel assembly but no effects on safety.

4. CONCLUSIONS

This paper presents the neutronic analysis of fuel design for a long-life core in a pressurized water reactor made of composite fuels, (including UN- 30 wt. % U_3Si_2 and 33 vol. % UO_2 -UN), and SiC cladding in comparison to the uranium oxide fuel UO_2 . It is found that use of the fuel of 15 % wt. U-235 of UO_2 , 15 % wt. U-235 of UNO, and 17.5 % wt. U-235 of UNSi,

with $P/D = 1.27$ and 1.0 to 2.5 % of Erbium as burnable poison addition makes it possible to design a PWR fuel that achieves high burnup. The fuel temperature coefficient of reactivity and both small and large void reactivity coefficients of the fuel designs are negative along fuel cycle with the concerned burnup target, 100 GWd/t burnup without compromising the safety parameters.

In the future study, this preliminary study would be refined and extended including full-core coupled neutronic-thermal-hydraulic analysis, stability analysis, transients and accidents analysis, as well as economic analysis. Furthermore, how to make use of the once-through burning fuel for energy production with employing fuel reprocessing would be considered in further study.

Data Availability

Data will be available upon request.

Conflict of interest

All authors declare no conflict of interest.

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Table I. Parameters of the fuel cells and assembly

Parameters	Reference	New design
Fuel diameter	0.8192	0.8192
Clad inside diameter, [cm]	0.8357	0.8357
Clad outside diameter, [cm]	0.9500	1.0357
Lattice pitch, P, [cm]	1.2598	Variables
P/D, [-]	1.3262	Variables
Equivalent pin pitch, [cm]	--	1.3118
Equivalent P/D, [cm]	--	1.2666
Rod array, [-]		17x17
Assembly pitch, [cm]	21.5	Variables
Linear heat rate, [W/cm]		176.5
Average coolant temperature in core, [K]		576.5
System pressure, nominal, [Mpa]		15.5
Average temperature for fuel, [K]		950.0
Average temperature for clad, [K]		607.0

Table II. Fuel cell selected characteristics versus P/D and U-235 enrichment.

Enrichment [wt. %]	Max. burnup, [GWd/t]			P/D for burnup \geq 100 GWd/t			k-inf at BOC, [-]		
	UNO	UNSi	UO ₂	UNO	UNSi	UO ₂	UNO	UNSi	UO ₂
4.45	--	--	30.0	--	--	--	--	--	1.3950
5.00	40.0	40.0	40.0	--	--	--	--	--	--
10.00	80.0	82.5	80.0	--	--	--	--	--	--
15.00	> 120	> 120	> 120	1.25-1.95	1.35-2.05	1.25-1.85	1.5224-1.6984	1.5624-1.700	1.5368-1.6959
17.50	> 120	> 120	--	1.15-1.95	1.15-2.05	--	1.4789-1.7151	1.4731-1.7143	--
20.00	> 120	> 120	> 120	1.15-2.05	1.25-2.05	1.15-1.95	1.4977-1.7268	1.5420-1.7251	1.5062-1.7265

Table III. Fuel cell and fuel assembly selected characteristics for various fuel compositions.

% Er2O3	15 wt. % - UO2				15 wt. % - UNO				17.5 wt. % - UNSi			
	k-inf at BOC		Max. burnup	PPF	k-inf at BOC		Max. burnup	PPF	k-inf at BOC		Max. burnup,	PPF
	Fuel cell	FA	[GWd/t]		Fuel cell	FA	[GWd/t]		Fuel cell	FA	[GWd/t]	
0.0	1.5568	1.5805	--	--	1.5394	1.5639	--	--	1.5357	1.5653	--	--
0.5	1.4770	1.5015	--	--	1.4693	1.4939	--	--	1.4821	1.5076	--	--
1.0	1.4145	1.4389	--	--	1.4138	1.4380	--	--	1.4388	1.4607	--	--
1.5	1.3631	1.3870	100.0	1.090	1.3678	1.3912	100.0	1.090	1.4023	1.4212	110.0	1.091
2.0	1.3194	1.3426	100.0	1.090	1.3285	1.3511	97.5	1.091	1.3707	1.3870	110.0	1.091
2.5	1.2814	1.3038	100.0	1.091	1.2941	1.3159	97.5	1.092	1.3428	1.3568	110.0	1.091
3.0	1.2478	1.2694	97.5	1.091	1.2636	1.2845	95.0	1.092	1.3178	1.3296	--	--
3.5	1.2175	1.2382	97.5	1.092	1.2360	1.2560	92.5	1.092	1.2949	1.3048	--	--
4.0	1.1899	1.2098	95.0	1.092	1.2108	1.2300	95.0	1.092	1.2740	1.2821	--	--
4.5	1.1645	--	--	--	1.1875	--	--	--	1.2545	--	--	--
5.0	1.1410	--	--	--	1.1659	--	--	--	1.2362	--	--	--
5.5	1.1191	--	--	--	1.1456	--	--	--	1.2190	--	--	--
6.0	1.0984	--	--	--	1.1266	--	--	--	1.2028	--	--	--
6.5	1.0790	--	--	--	1.1085	--	--	--	1.1873	--	--	--
7.0	1.0605	--	--	--	1.0914	--	--	--	1.1725	--	--	--
7.5	1.0430	--	--	--	1.0751	--	--	--	1.1584	--	--	--
8.0	1.0263	--	--	--	1.0594	--	--	--	1.1447	--	--	--

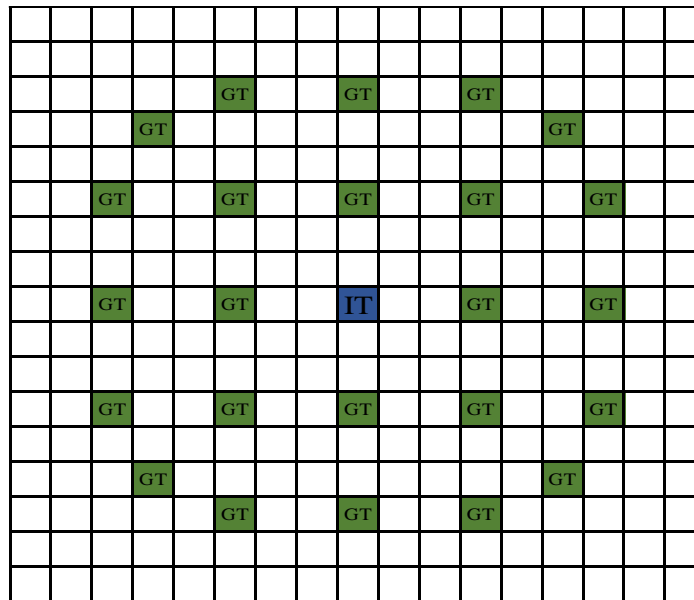


Fig. 1. Layout of fuel assembly (GT: guide thimbles; IT: instrumentation thimble; others: Fuel rods).

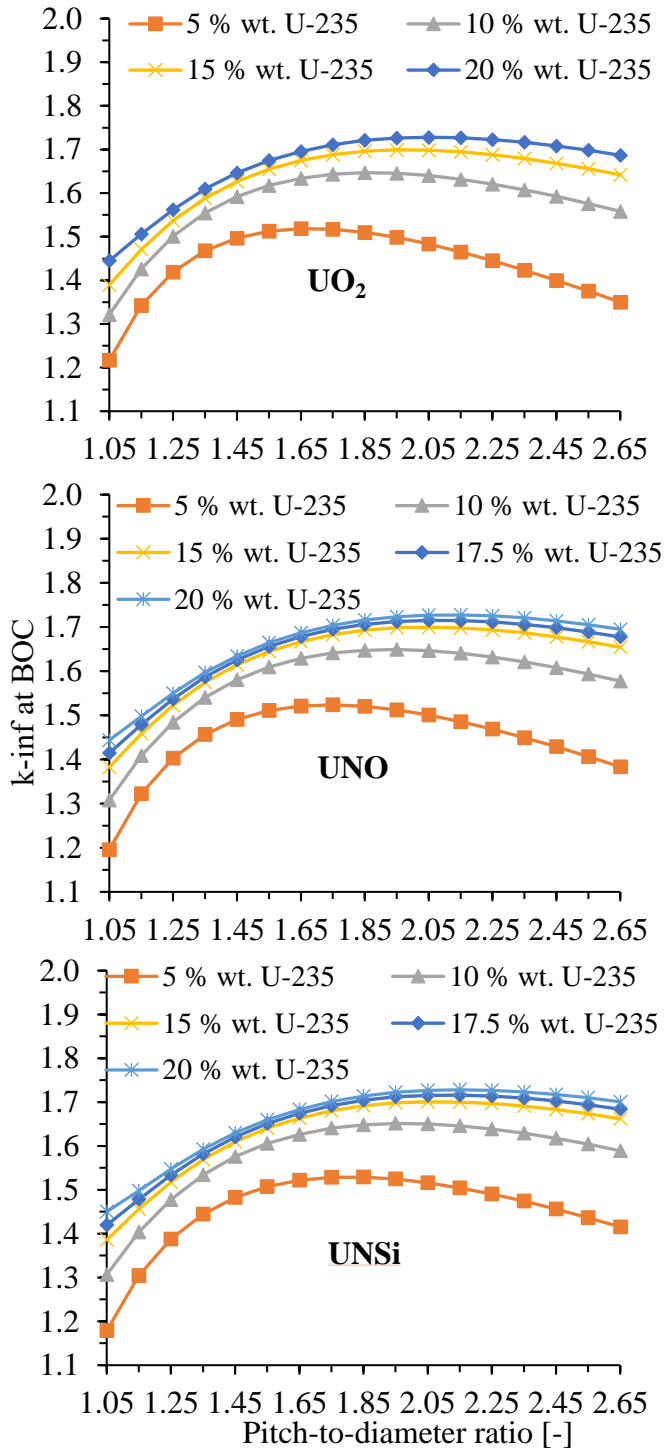


Fig. 2. k_{inf} at BOC as a function of P/D

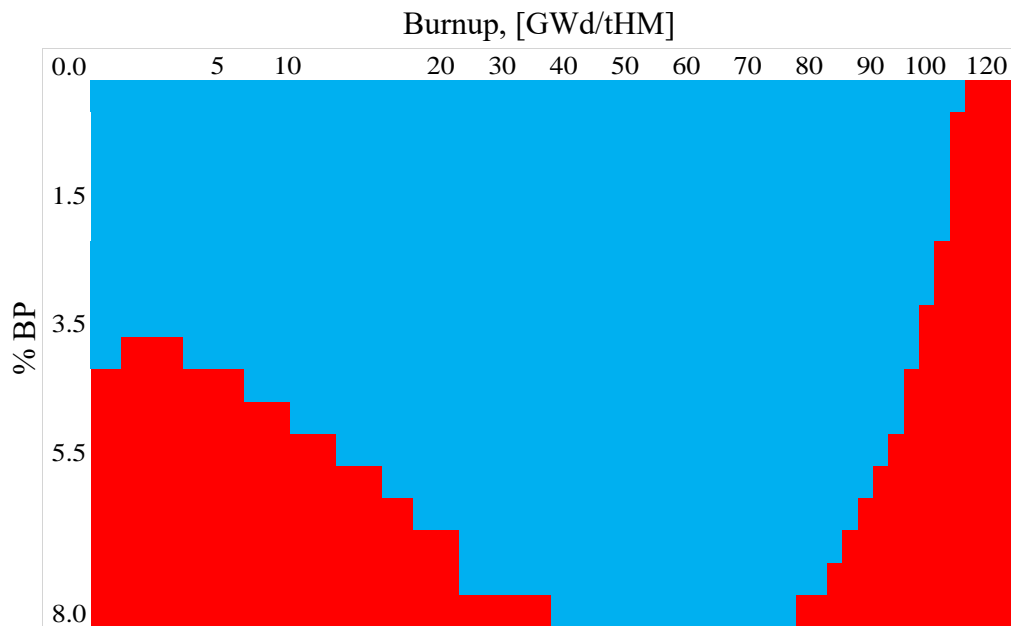


Fig. 3. Design space of UO_2 fuel cell loaded 15 % U-235 enrichment fuel with BP

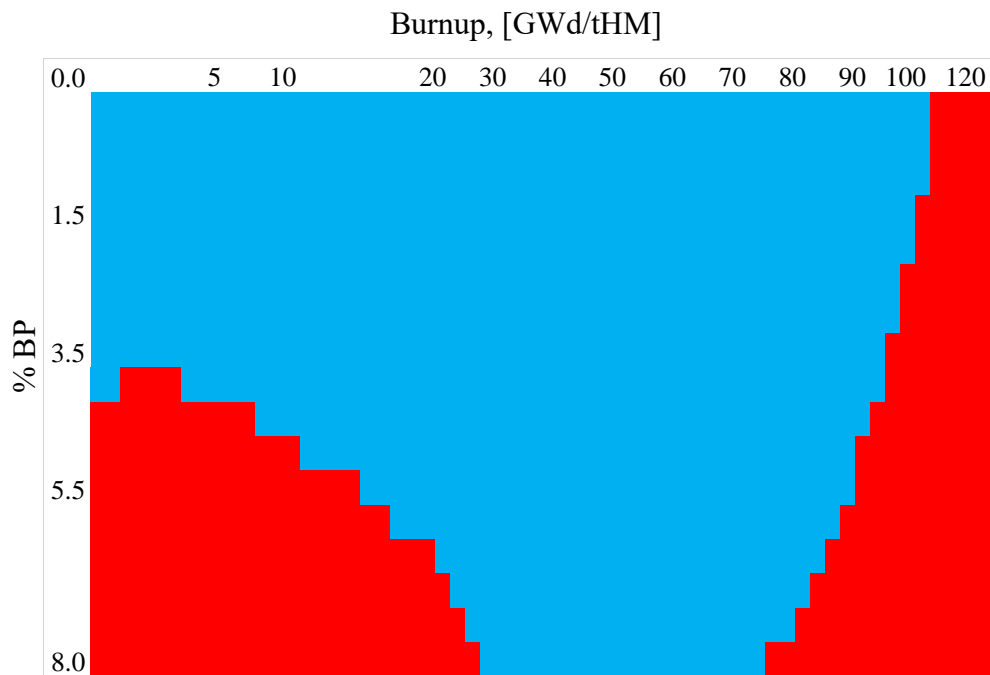


Fig. 4. Design space of UNO fuel cell loaded 15 % U-235 enrichment fuel with BP

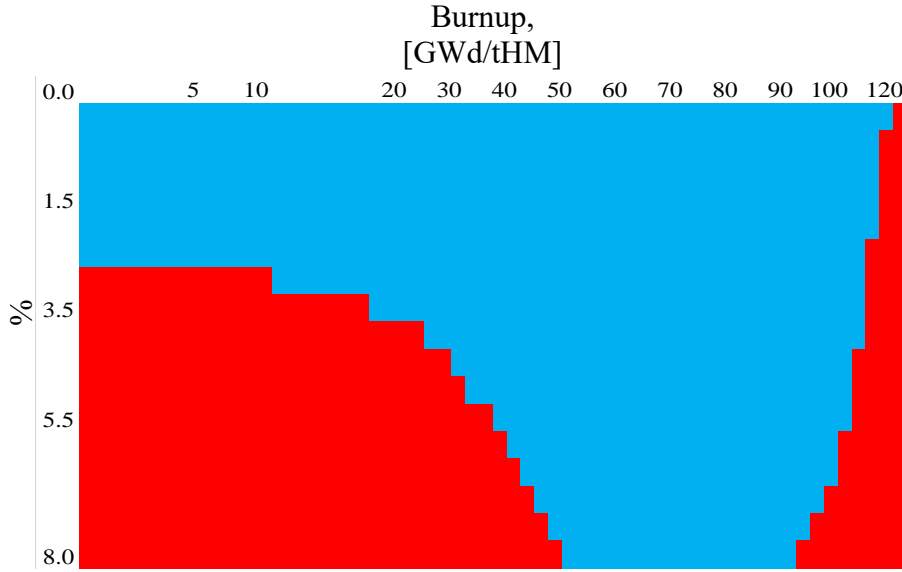


Fig. 5. Design space of UNSi fuel cell loaded 17.5 % U-235 enrichment fuel with

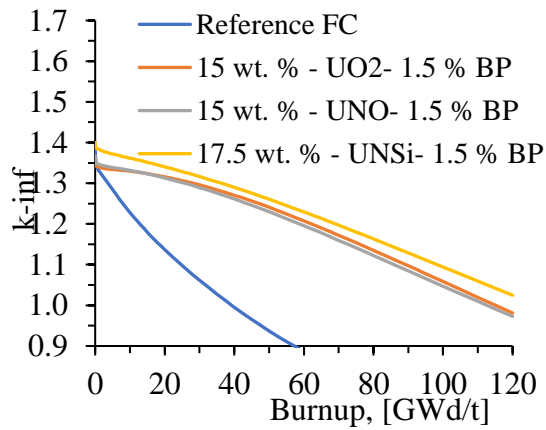


Fig. 6. K-infinity variation with burnup

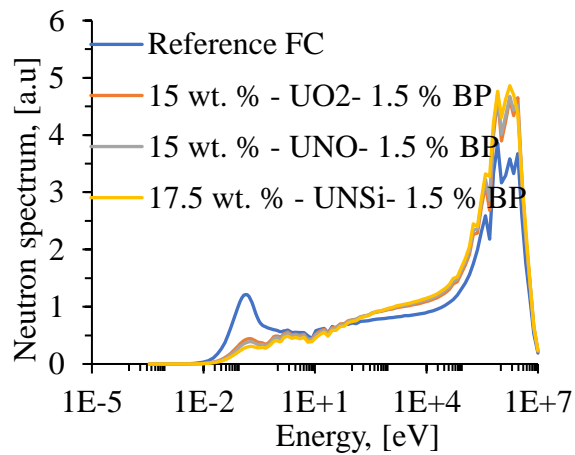


Fig. 7. Neutron flux per lethargy at BOC

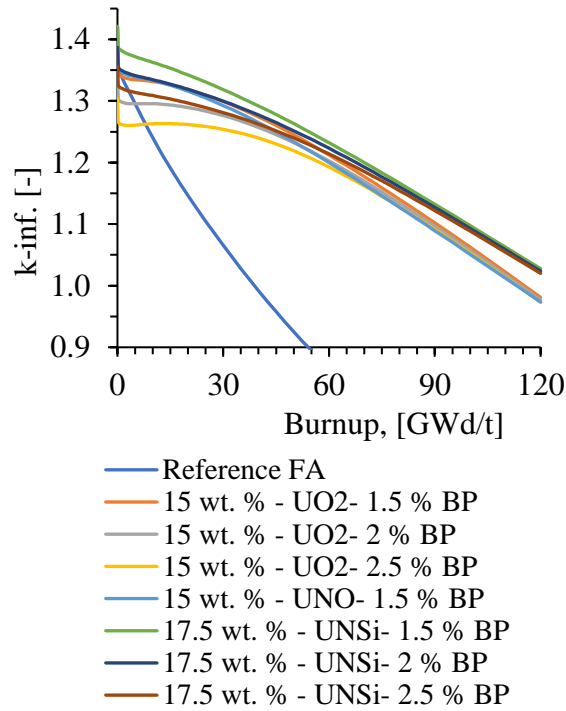


Fig. 8. K-infinity of FAs versus burnup

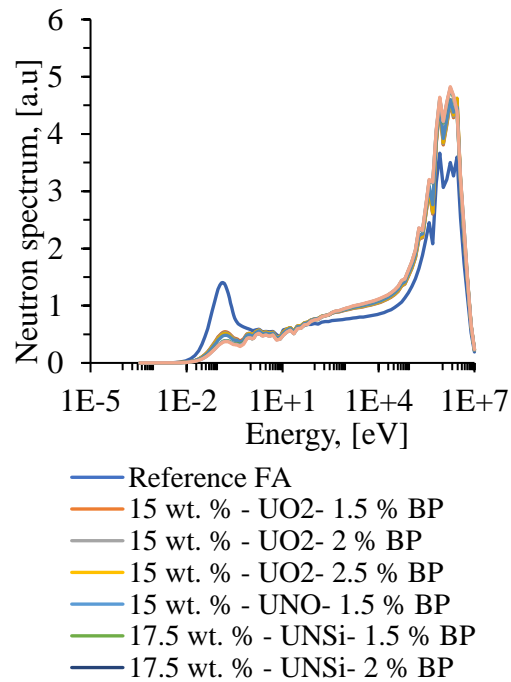


Fig. 9. Neutron flux per lethargy of FAs at BOC