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# Effective multiplication factor and fuel temperature coefficient calculations of PWR assembly under different temperatures

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#### Abstract

This paper presents effective multiplication factor  $(k_{eff})$  with different burnable absorbers and weight percentages at different temperatures as well as doppler coefficient results and number density calculations for Westinghouse type pressurized water reactor (PWR) Assembly. Integral fuel burnable absorber rods coated with ZrB<sub>2</sub> and Gadolinia-Uranium (UO<sub>2</sub>-Gd<sub>2</sub>O<sub>3</sub>) integral burnable absorbers were considered to calculate reactor parameters ( $k_{eff}$  and doppler coefficient). The results compared with base fuel which does not contain burnable absorber at different temperatures. The results show that reactivity was decreased with increased temperature and doppler coefficients increased with temperatures but remained negative at all temperatures. At 1500 K, the effective multiplication factor for base fuel was found to be 1.46985 while the effective multiplication factors for 2% with Gd<sub>2</sub>O<sub>3</sub>, 8% with Gd<sub>2</sub>O<sub>3</sub>, and IFBA rods were 1.38976, 1.37574, and 1.30337 respectively.

Keywords: Burnable absorber, Doppler coefficient, reactor parameters, fuel assembly.

# Farklı sıcaklıklar altında BSR yakıt demetinin efektif çoğalma faktörü ve yakıt sıcaklığı katsayısı hesaplamaları

### Özet

Bu çalışmada, Westinghouse tipi basınçlı su reaktörü (BSR) yakıt demeti için, çeşitli sıcaklıklarda farklı yanabilir zehirler ve ağırlık yüzdeleri kullanılarak efektif çoğalma faktörü ( $k_{eff}$ ), doppler katsayı sonuçları ve yoğunluk hesaplamaları sunulmaktadır. Reaktör parametreleri olan  $k_{eff}$  ve doppler katsayıları, ZrB<sub>2</sub> ile kaplanmış integral yakıtlı yanabilir zehir çubukları ve Gadolina-Uranyum (UO<sub>2</sub>-Gd<sub>2</sub>O<sub>3</sub>) integral yakıtlı

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yanabilir zehirler göz önüne alınarak hesaplanmıştır. Farklı sıcaklıklarda elde edilen sonuçlar, yanabilir zehiri kullanılmayan yakıt demeti sonuçları ile karşılaştırılmıştır. Artan sıcaklık değerlerinde, yakıt demetlerinde reaktiflik azalmış doppler katsayıları ise artmıştır fakat doppler katsayıları her sıcaklıkta negatif değerlerde kalmıştır. Sıcaklığın 1500 K'de olduğu durumda yanabilir zehirli olmayan temel yakıt demetinde efektif çoğalma faktörü 1.46985 iken ağırlık yüzdesi %2 ve %8 olan  $Gd_2O_3$  ile IFBA yanabilir zehirli yakıt demetinin efektif çoğalma faktörü sırasıyla 1.38976, 1.37574 ve 1.303370larak bulunmuştur.

Anahtar Kelimeler: Yanabilir zehir, Doppler katsayısı, reaktör parametreleri, yakıt demeti.

#### **1. Introduction**

Researchers have been developed many different absorber materials to increase the cycle length of reactor core [1]. Burnable absorbers have been used in nuclear fuel of light water reactors (LWRs) since they increase the length of cycle in the core. One of the important selection criteria for burnable absorber material is to hold down excess reactivity at the beginning of cycle. Another desirable material property for selection of burnable absorber is to maximize the cross section for slow neutrons at beginning of nuclear fuel cycle. For pressurized water reactor (PWR), reactivity decreases linearly with respect to burnup if there is no burnable absorber in the fuel assemblies. Therefore, some PWR nuclear fuel assemblies such as Westinghouse PWR contain integral fuel burnable absorber (IFBA) rods, which load with uranium dioxide (UO2) pellets coated with ZrB2 to control reactivity in the core. In addition, fuel rods with Gadolinia-Uranium (UO2-Gd2O3) integral burnable absorber have been used broadly in boiling water reactors (BWRs) for reactor control and effective fuel performance [2]. Gadolinia integral burnable absorber provides high thermal neutron cross section but gadolinium in the fuel decreases the thermal conductivity and melting point of uranium. Thermal neutron absorption cross section and natural abundance of gadolinium (Gd) isotopes is much higher than Boron-10 isotope [3].

In a nuclear reactor, the cross sections of neutrons or the interaction probability with nuclear fuel nucleus depend mostly on the temperature. Thermal motion of nucleus alters because of fuel temperature fluctuation. It has been observed that as fuel temperature rises, the resonance in the interaction probability widens while its magnitude of the peak reduces. This event is called as Doppler Effect [4]. The fuel temperature coefficient (FTC) of reactivity or Doppler coefficient is an essential parameter in a nuclear reactor core assessment. The FTC assessment contains the reactivity change with fuel temperature change by keeping other parameters such as burnup, moderator density, boron concentration, moderator temperature [5].

In this study, application of MCNP (Monte Carlo N-Particle) code on 17x17 Westinghouse PWR Assembly is performed to calculate reactivity and FTC (Doppler coefficient) with various weight percent of burnable poisons at different temperatures. Additionally, the density of fuel compositions were calculated based on selected material weight percentages.

#### 2. Methods and compositions of fuel assemblies

The reactivity and Doppler coefficient calculations with IFBA rods, Gadolinia rods and without burnable absorbers were implemented using MCNP code. A 17x17 Pressurized Water Reactor Assembly, which includes 25 water rods, has been selected for reactivity and Doppler coefficient calculations at five different temperatures (300 K, 600 K, 1000 K, 1200 K and 1500 K). Fuel assembly with five percent enriched UO<sub>2</sub> fuel and 25 water rods is considered to be base fuel as shown in Figure 1. The base fuel input deck was modified to accommodate the addition of IFBA rods that has a thin  $ZrB_2$  layer with 55% enriched <sup>10</sup>B.  $ZrB_2$  coating at specified 2.4 mg <sup>10</sup>B per 2.54 cm added to input deck for preparation of the 80 IFBA rod case. The thickness of the coating added to the fuel pellet is calculated for the specified 2.4 mg <sup>10</sup>B per 2.54 cm as shown in Figure 3. The elaborated density calculations of fuel composition were obtained to find the coating thickness.



Figure 1. Base fuel assembly.

For the case of Gadolinia-Uranium ( $UO_2$ -Gd<sub>2</sub>O<sub>3</sub>) burnable absorber, the fuel assemblies were created by substituting of <sup>235</sup>U, <sup>238</sup>U, <sup>16</sup>O and varying amounts of 2, 4, 6, and 8 weight percent of Gd isotopes into eight fuel rods as shown in Figure 2. Note that the amount of gadolinium is specified as weight percent of the metal gadolinium of various isotopes in the form of gadolinia mixed with UO<sub>2</sub>. The theoretical density (TD) of UO<sub>2</sub> with gadolinia is given as [6];

$$Density(\rho) = 10.96 - 0.033.(Gd_2O_3\%)$$
(1)

The number densities for each material within a specified concentration of  $Gd_2O_3$  are calculated. These number densities were used in the MCNP program to be able to calculate reactivity and Doppler coefficients. After creating libraries by compiling NJOY99 program at different temperatures (300 K, 600 K, 1000 K, 1200 K and 1500 K), the MCNP simulations were completed for base fuel and modified assemblies with  $Gd_2O_3$  and  $ZrB_2$  burnable poison rods.

After the  $k_{eff}$  with respect to temperature plot with all fuel composition MCNP runs, the multiplicative value before the logarithmic function will provide the Doppler constant of a particular fuel assembly. This shows the fuel reactivity and changes of the reactivity in

temperature. It is expected this value is negative because of the U-238 Doppler coefficient. It is absorbing more neutrons at the different temperatures. If the  $k_{eff}$  value is close to 1, the fuel temperature coefficient  $\alpha_{\tau}$  can be calculated as [7],

$$\alpha_T = \frac{1}{k_{eff}} \frac{\partial k_{eff}}{\partial T}$$
(2)

If the  $k_{eff}$  value is not close to 1, the fuel temperature coefficient  $\alpha_{\tau}$  can be calculated as [7],

$$\alpha_T = \frac{1}{k_{eff}^2} \frac{\partial k_{eff}}{\partial T}$$
(3)



Figure 2. The fuel assembly with gadolinia-uranium (UO<sub>2</sub>-Gd<sub>2</sub>O<sub>3</sub>) burnable absorber.

#### **3. Results and discussions**

The modifications of the 80 IFBA rods were same with  $Gd_2O_3$  addition but the difference was the new surface card addition. A new universe created for the fuel assembly and cell card modified for a new surface that made up space in the air gap between the cladding and the fuel.

To figure out the radial distance from the centerline of the fuel to the edge of the  $ZrB_2$  coating the new surface card was created. The  $ZrB_2$  coating added at the specified 2.4 mg <sup>10</sup>B per inch and the thickness of coating was calculated to be approximately 0.000615 cm as shown in table 1. The cross-sectional view and magnified of coating view of IFBA rods were provided in Figure 3. The total Boron mass for single IFBA rod with 388.1 cm long and 55% enriched <sup>10</sup>B was obtain 0.3667 g. Therefore, the total boron mass in one single assembly can be calculated as 29.336 g.

The calculated number densities for each fuel composition were used in input decks. The calculated number densities tabulated in Table 2 and 3. The density calculations showed that the density of Gd isotopes with the variation of weight percentage was increased while the number densities of U and O isotopes were decreased.



Figure 3. IFBA rods with thin ZrB<sub>2</sub> layer and 55% enriched <sup>10</sup>B and magnification of coating view.

Number of IFBA rods	80
Length of rod (cm)	388.1000
Length rod (inch)	152.7953
Diameter of fuel pellet (cm)	0.8190
Surface area of per rod (cm <sup>2</sup> )	2.5730
Circumference of fuel pellet (cm)	998.5675
Mass ZrB <sub>2</sub> /IFBA rod	55 wt%
Mass B10/inch/IFBA rod (g)	0.0024
Mass B10/IFBA rod (g)	0.3667
Density $ZrB_2$ (g/cc)	3.7446
Surface area of per rod (cm <sup>2</sup> )	6.0900
Radius of pellet (cm)	0.4095
Thickness ZrB2 (cm)	0.00061575
Distance from center to edge of ZrB <sub>2</sub>	0.41011570

Table 1: Thickness of the coating added to the fuel pellet for IFBA rods.

Table 2: Densities of Gd<sub>2</sub>O<sub>3</sub> and UO<sub>2</sub>.

Densities	8 wt% Gd	6 wt% Gd	4 wt% Gd	2 wt% Gd
$Gd_2O_3$ (g/cc)	0.98116796	0.74143187	0.49799184	0.25084789
$UO_2$ (g/cc)	9.65948228	9.97955581	10.30333327	10.63081467
Total (g/cc)	10.64065024	10.72098768	10.80132512	10.88166256

The simulations were completed for all 6-fuel schemes, which provide 30 input files, at 300 K, 600 K, 1000 K, 1200 K and 1500 K to find out reactivity change and Doppler coefficient with respect to temperature increase. The simulated data was analyzed and the graph of the  $k_{eff}$  values with respect to temperature for the six fuel types plotted in Figure 4. The figure describes that the  $k_{eff}$  value decreases when the temperature increases. It is also indicate that the  $k_{eff}$  decreases by adding more burnable absorbers. For consistency reasons, effective multiplication factors ( $k_{eff}$ ) were observed for UO<sub>2</sub> base fuel and gadolinia mixed fuel (UO<sub>2</sub>-Gd<sub>2</sub>O<sub>3</sub>). The effective multiplication factor,

which effects the reactivity results for  $UO_2$  base fuel and gadolinia mixed fuel ( $UO_2$ -Gd<sub>2</sub>O<sub>3</sub>) are 1.47688 and 1.38989 with standard deviation of 0.00059 and 0.00062 at 1200 K, respectively.

Isotopo	Number Density (atoms/mol)				
Isotope	8 wt% Gd <sub>2</sub> O <sub>3</sub>	6 wt% Gd <sub>2</sub> O <sub>3</sub>	$4 \text{ wt\% } \text{Gd}_2\text{O}_3$	$2 \text{ wt\% } Gd_2O_3$	
Gd-154	7.10665E+19	5.37023E+19	3.60698E+19	1.8169E+19	
Gd-155	4.82470E+20	3.64584E+20	2.44877E+20	1.23349E+20	
Gd-156	6.67308E+20	5.04259E+20	3.38692E+20	1.70606E+20	
Gd-157	5.10179E+20	3.85523E+20	2.58941E+20	1.30434E+20	
Gd-158	8.09767E+20	6.11910E+20	4.10997E+20	2.07027E+20	
Gd-160	7.12621E+20	5.38501E+20	3.61691E+20	1.82190E+20	
O-16	4.78597E+22	4.8092E+22	4.83224E+22	4.85508E+22	
U-235	1.55102E+20	1.60242E+20	1.65441E+20	1.70699E+20	
U-238	2.13857E+22	2.20944E+22	2.28112E+22	2.35362E+22	
TOTAL	7.26540E+22	7.28051E+22	7.29503E+22	7.30895E+22	

Table 3: Number	densities with	percent of	gadolinia	absorber	(UO	$2-Gd_2$	$O_3$	).
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The fuel temperature coefficients were calculated based on Eq. (3). Fuel temperature 300 K was considered as the reference temperature for all FTC calculations and unknown value of  $\partial k_{eff}$  was obtained by subtraction of  $k_{eff}$  values for different temperatures. This leads to Doppler coefficient for each individual cases using the all known values. The results from the equations can be seen in Table 4 where fuel temperature coefficient is always stays negative and increase with increased temperatures but after 1200 K it is decrease.



Figure 4. k<sub>eff</sub> change with respect to temperature for each fuel type.

Fuel Form	Temperature (K)	k <sub>eff</sub>	$\partialk_{eff}$	$\alpha_T$ ,Fuel temp. coefficient $(\Delta k/k)$
Base case	300	1.50587	-	-
Base case	600	1.49430	-0.01157	-2.45514E-05
Base case	1000	1.48129	-0.01301	-1.48425E-05
Base case	1200	1.47688	-0.00441	-1.24023E-05
Base case	1500	1.46985	-0.00703	-9.95491E-06
$2 \text{ wt \% } Gd_2O_3$	300	1.42288	-	-
$2 \text{ wt \% } Gd_2O_3$	600	1.41139	-0.01149	-2.48392E-05
$2 \text{ wt } \% \text{ Gd}_2\text{O}_3$	1000	1.40085	-0.01054	-1.50178E-05
$2 \text{ wt } \% \text{ Gd}_2\text{O}_3$	1200	1.38989	-0.01096	-1.25492E-05
$2 \text{ wt \% } Gd_2O_3$	1500	1.38976	-0.00013	-1.00732E-05
4 wt % Gd <sub>2</sub> O <sub>3</sub>	300	1.41645	-	-
4 wt % Gd <sub>2</sub> O <sub>3</sub>	600	1.40546	-0.01099	-2.37069E-05
4 wt % Gd <sub>2</sub> O <sub>3</sub>	1000	1.39362	-0.01184	-1.43282E-05
4 wt % Gd <sub>2</sub> O <sub>3</sub>	1200	1.38952	-0.00410	-1.19715E-05
4 wt % Gd <sub>2</sub> O <sub>3</sub>	1500	1.38350	-0.00602	-9.60798E-06
$6 \text{ wt } \% \text{ Gd}_2\text{O}_3$	300	1.41277	-	-
$6 \text{ wt } \% \text{ Gd}_2\text{O}_3$	600	1.40076	-0.01201	-2.25955E-05
$6 \text{ wt } \% \text{ Gd}_2\text{O}_3$	1000	1.39077	-0.00999	-1.36519E-05
$6 \text{ wt } \% \text{ Gd}_2\text{O}_3$	1200	1.38578	-0.00499	-1.14049E-05
$6 \text{ wt } \% \text{ Gd}_2\text{O}_3$	1500	1.38054	-0.00524	-9.15189E-06
8 wt % $Gd_2O_3$	300	1.40863	-	-
8 wt % $Gd_2O_3$	600	1.39733	-0.01130	-2.38596E-05
8 wt % $Gd_2O_3$	1000	1.38708	-0.01025	-1.44212E-05
8 wt % $Gd_2O_3$	1200	1.38404	-0.00304	-1.20494E-05
8 wt % $Gd_2O_3$	1500	1.37574	-0.00830	-9.67070E-06
80 IFBA Rods	300	1.33308	-	-
80 IFBA Rods	600	1.32206	-0.01102	-2.27126E-05
80 IFBA Rods	1000	1.31282	-0.00924	-1.37231E-05
80 IFBA Rods	1200	1.30980	-0.00302	-1.14646E-05
80 IFBA Rods	1500	1.30337	-0.00643	-9.19990E-06

Table 4: Fuel temperature coefficient.

<sup>238</sup>U resonances widen so that increases the neutron absorption. This leads to reactivity reduction in the core. As it is known LWRs contains low enriched uranium fuel, which contains huge amount of <sup>238</sup>U, therefore, the Doppler broadening is expected to be higher. Figure 5 shows that fuel temperature coefficients is negative for all temperature range under consideration. The FTCs are increasing almost linearly until 1200 K including within the operating temperature of a PWR (563 K - 623 K) and decreases after this temperature decreases for burnable poison cases. However, the FTC of base fuel is still increasing until 1500 K. It is important to note that, when FTC is negative (for reactor operation temperatures) then  $\partial k/\partial T$  must be negative. Therefore, increased temperature cases the reactivity values decrease. The FTC with a positive value for a reactor is intrinsically unstable to changes in its temperature but reactor with a negative FTC is stable [8].



Figure 5. Fuel temperature coefficient change with respect to temperature for each fuel type.

#### 4. Conclusion

In this study, reactivity change and fuel temperature coefficient of  $ZrB_2$  and  $Gd_2O_3$  were obtained at various temperatures using MCNP simulations. Number densities were calculated to obtain necessary simulations. The thickness of ZrB<sub>2</sub> coating were calculated 0.000615 cm at 2.4 mg<sup>10</sup>B per inch. It has been observed that reactivity decreases with temperature increase. Besides, the reduction of reactivity depends on selection of burnable absorber and weight content. At 300 K, the reactivity for base fuel is 1.50587 while the reactivity for 2% with  $Gd_2O_3$  and 8% with  $Gd_2O_3$  rods is 1.42288 and 1.40863, respectively. This indicates that adding more burnable absorber in the fuel rod leads to high neutron absorption, which eventually result in reactivity decrease. On the other hand, at same temperature, the reactivity of IFBA rods with ZrB<sub>2</sub> coating is 1.33308, which proves that various burnable absorbers may effect differently in reactivity. Finally, fuel temperature coefficients calculated based on Eq. (3) for each fuel type including base fuel as shown Figure 5. The temperature coefficients for all fuel types were increased with temperature until 1200 K but remained negative. The Doppler coefficient of most thermal reactors is negative because of the nuclear Doppler Effect, which decreases the magnitude of absorption cross section if the temperature increases. This will lead to increase the average flux in the resonance, eventually reduce the reactivity in the core [8].

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