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Investigation of Thorium Utilization in a New SMR Core Design

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Abstract. Thorium is considered to be a key element in future nuclear technology because of huge amount of reserves in the world. Several investigations have been performed by many of researcher groups around the world for Th-U breeding including the ones in Turkey. In addition, Turkey has one of the biggest thorium reserves in the world, therefore it is important to work on Th utilization for Turkey's reactors. Small modular reactors (SMRs) are standardized, easy to construct and inherently safe new innovative designs. Because of these, a new core design of an SMR is performed in this study. The aim of the study is to determine the basic cell configuration and maximum ^{232}Th to ^{233}U conversion with most promising SMR design parameters and to reach conversion ratio up to 1. In this study, criticality and burnup calculations were performed with MCNP6.1.1 code system which includes CINDER burnup module with newly generated cross-section sets by NJOY99. Heterogeneous core design (axial pellet type variation or pin based designs) was performed since it is important for neutronic aspects when thorium is added to the nuclear reactor fuel to increase conversion. To this respect, 3D pincell simulations were performed for different heterogeneous neutronic design cases.

Keywords: Burnup, Conversion, MCNP, SMR, Thorium

1 Introduction

Due to increasing energy need in the globalizing world, more energy production requirement has emerged. In order to overcome this energy requirement, the developed and developing countries have taken preventive measures such as increasing quantity of electrical energy resources and improving the existing ones, and finding new energy sources

Turkey is a developed country with %2.3 gross domestic product (GDP) [1] and requires much more energy with increasing GDP. Turkey has decided to construct two large nuclear reactors on the northern and southern coastal regions by 2023 to compensate the increasing electrical need every passing year.

According to the classification currently adopted by IAEA, small reactors are the reactors with an equivalent electric power less than 300 MW, medium sized reactors are the reactors with an equivalent electric power between 300 and 700 MW. Small reactors came first historically, as power sources for nuclear submarines [2]. In recent years, Small Modular Nuclear Reactor (SMR) technology has become one of the most popular technology issues in the nuclear area. Since SMRs are inherently safe, able to be standardized and are easy and cheap to construct when they are compatible with the commercial reactors, they are very popular among nuclear reactor vendors, investigators and scientists. There are different SMR designs that were designed such as water cooled (specialized PWR and BWR), liquid metal cooled, molten salt etc. Except the water cooled ones, the other SMRs have huge unsolved engineering problems such as metallic corrosion, volatile gas evacuations etc. Probably the solution of these problems will not take longer time than expected.

Alongside of the unresolved problems, SMRs need more enriched (approximately 10-20% by mass of fuel) uranium than current commercial nuclear reactors. Although higher enrichment is limited by the international laws, increased enrichment levels provide higher burnup values than commercial reactors.

One of the important aspects in the future nuclear technology is the fast breeding nuclear reactor (FBR) technology in the world. Projections show that ^{235}U amount will be not enough in the future, such that uranium resources can be adequate 50 years in the world [3]. In many countries, FBR technology investigation has been continued regularly.

Another important aspect when it comes to dealing with the decrease in available uranium amount is that using thorium as a nuclear fuel in future reactors. Thorium (^{232}Th) is not a fissile element and cannot undergo fission reaction by itself. However, ^{232}Th can be converted to ^{233}U; ^{233}U is a fissile element and undergoes fission reaction. The Th-U breeding is planned as a three stages program by the Indian Government to convert fertile element ^{232}Th to fissile ^{233}U in breeder reactors and perpetually continuation the ^{233}U production.

Taking the above listed considerations into account, i.e. SMRs, FBRs and ^{232}Th conversion, combination of these considerations may be an important aspect in developing nuclear technology in Turkey, since Turkey has one of the biggest thorium reserves in the world and it is a new comer country that wants to build and operate its own reactors in the future.

For these reasons, initiation of a new core design of an SMR is performed in this study. Determination of basic cell configurations and maximizing ^{232}Th to ^{233}U conversion is investigated. To perform basic criticality and burnup calculations, MCNP6.1.1 [4] code system and newly generated cross-section sets generated by NJOY99 are used. To increase conversion in the nuclear fuel element, axial pellet type variation in pin based design was performed.

2 Why Thorium?

All commercial nuclear reactors have used Uranium dioxide as the fuel in the world. According to NEA Red Book, annular uranium requirement is 61600 tU for 437 nuclear power plants [5]. In addition, if more than 60 reactors that are under construction all around the world is considered, existing uranium reserves will not be sufficient and different type of nuclear fuel investigations will be required in the future.

As mentioned above, thorium in not a fissile element itself and it does not undergo fission reaction in thermal and epithermal neutron energy ranges. However, if ^{232}Th absorbs a neutron and transmutes to ^{233}U, the new transmuted element ^{233}U will be a fissile element and it can undergo fission event easily. At this point, a crucial question immediately comes in the human mind, “Why we do not use ^{238}U as a fertile material to generate fissile ^{239}Pu, although it has enough abundance in the world?” It can be true but we consider very comprehensively given in the following:

- We should be worried about the future availability of nuclear energy sources.
- Proliferation issue is an important topic for nuclear related areas. Building a nuclear weapon from ^{233}U is rather resistive than ^{235}U and ^{239}Pu.
- In reactor operation, neutron multiplication properties of ^{233}U and ^{232}Th make it easier to achieve negative void reactivity coefficient due to less steep dependence of ^{233}U η-factor on energy compared to ^{239}Pu in fast spectrum
- Smaller fast fission cross-section of ^{232}Th compared to ^{238}U. [6].

Less waste and control mechanism due to maximized fertile capture.

For breeding, thorium is also investigated due to valuable neutronic properties in thermal and epithermal energy regions. It is presented in Figure 1 that thorium absorption cross section nearly three times greater than ^{238}U in thermal and epithermal energy regions. This condition increases fertile capture therefore fertile to fissile conversion ratio goes up.

When the neutron fission cross sections of ^{233}U and ^{235}U shown in Figure 2 are examined, one can see that, although fission cross sections are nearly the same for ^{233}U and ^{235}U, ^{239}Pu cross section is perceptibly higher than the others. Nevertheless, ^{235}U and ^{239}Pu cross sections are rapidly decreasing at the end of the epithermal and fast neutron energy spectrum, ^{233}U cross section is nearly stable and also shows increasing trend. That is why thorium breeding is very important in thermal and epithermal energy regions.

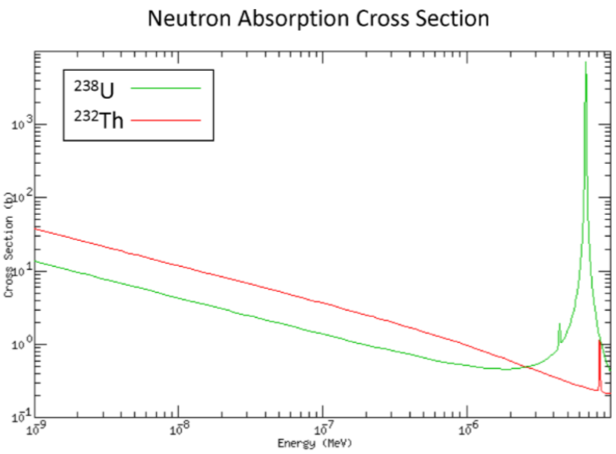

Figure 1. Neutron absorption cross section of ^{232}Th and ^{238}U.

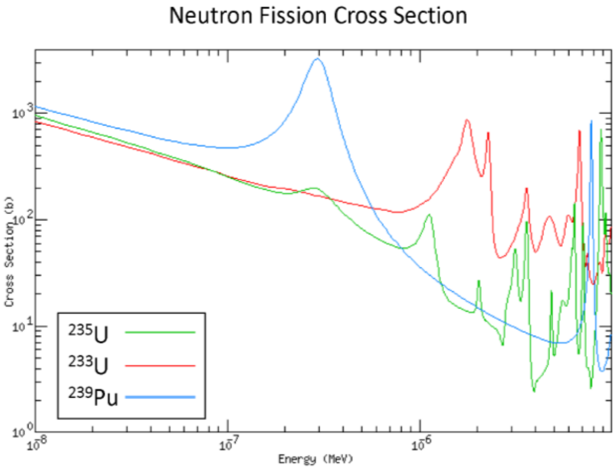

Figure 2. Neutron fission cross section of ^{233}U ^{235}U and ^{239}Pu.

In literature, there are a lot of work which include utilization of thorium for light water reactors. For example, *Mushakov and Morozhov* [7] have investigated Th-U mixed fuels in VVER reactor, *Ganda et al.* [8] has investigated the reduced moderation BWR that is a thorium-fuelled water-cooled reactor core design approach that features a radially uniform composition of fuel rods in stationary fuel assembly and its fuel-self-sustaining is described.

3 Calculation Procedure

3.1 Preparation of neutron cross sections

Effective neutron cross sections that are characterizing neutron behavior and target material interactions are important parameters in normal operation conditions and determination of safety limitations. These effective neutron cross sections depend on a lot of parameters such as isotopic composition of materials, fuel cell geometry, reactor operation temperatures, neutron energy spectrum, burnup, reactor type etc. Raw neutron data libraries (Evaluated Neutron Data File – ENDF) have been collected based on both experimental and theoretical results. However, Monte Carlo based codes such as MCNP and SCALE cannot use raw neutron libraries while simulating neutronic reactions. These type of codes are able to access A Compact ENDF (ACE) formatted files. If someone wants to convert these raw data libraries to ACE files, ENDF files can be converted by using NJOY99 [9,10] code.

In this work, we were generated all required neutron data libraries including proper material temperatures, Doppler broadening, heating kermas and probabilistic unresolved resonance calculations were generated with NJOY99.396 [9] code.

3.2 Designing a new core

In nuclear reactor design, main purpose of the designer is adjusting the temperature of materials which does not exceed the limitations in anywhere in the reactor core. This adjustment is made by changing the amount of fuel, reactor flow rate, operating conditions and heat transfer area. Core lattice structure is determined by considering nuclear, hydraulics and heat transfer options. In the next step which more detailed analysis is performed, all of nuclear, structural, material, hydraulics, heat transfer and economic performance analyses are considered.

When the heat transfer analysis is performed, the main objective is that heat flux does not exceed the critical heat flux and temperature limitations in the fuel element are not violated.

Determining the critical heat flux limitations, nuclear channel peaking factors are important parameters. As one of the first steps of core design, nuclear peaking factors and engineering hot channel factors are clearly defined by the designers. (These are determined a bit higher than real values to be conservative to stay in conservative region during any extraordinary operational condition. The basic design steps for a new reactor are describing in following subsections.

Determination of power output. The net electrical output in MW$_e$ is determined by the electric utility and by the grid requirements. In this work, it is aimed to design an SMR reactor core and, (for electrical output is not less than 300 MW$_e$), the electric output was as 300 MW$_e$.

Determination of the reactor type and basic parameters. In this work, the most important issue is to obtain the utilization of thorium. For this purpose, reactor fuel pitch is designed as tight as possible for conversion, since ^{232}Th absorption cross section is higher than the absorption cross section of ^{238}U in which neutron energy is higher than thermal neutron energies. Hexagonal pitch approximation provides very tight and regular sequence for conversion and cooling the fuel pins. In addition to conversion and cooling, the reactor design was determined by taking previously gained operating and practical experiences into account. Thus reactor type is determined as pressurized water reactor (PWR) having hexagonal pitch.

Overall thermal power is specified by assuming standard PWR plant efficiency. Hence thermal efficiency of the plant is taken as 33.3 % and thermal power of the reactor is 900 MW$_{th}$. After specifying reactor thermal power and engineering hot channel factors, hand calculations were performed for determination of core dimensions, fuel rod height and number of fuel rods by making square cylinder core approximation.

To define the most efficient pitch dimension for conversion, pitch size of the unit cell was changed from 10.0 mm to 12.75 mm with increment step size of 0.25 mm shown in Figure 3. To determine the best axial location for the ^{232}Th pellets, a Python® [11] script was written which automatically prepares the MCNP inputs. Figure 4 presents

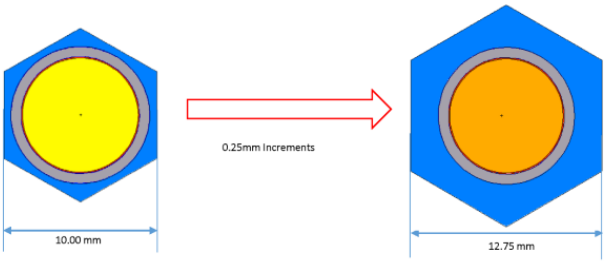

Figure 3. Pitch dimension changes.

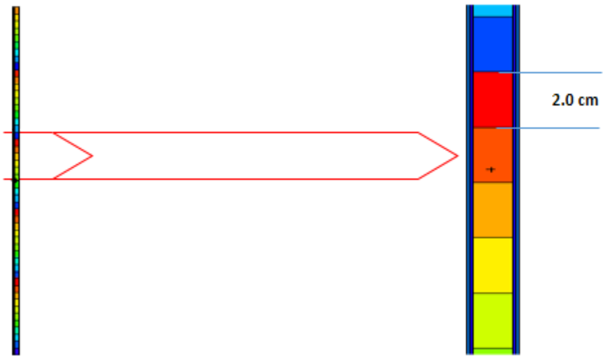

Figure 4. Axial cross section of pellets in fuel pin.

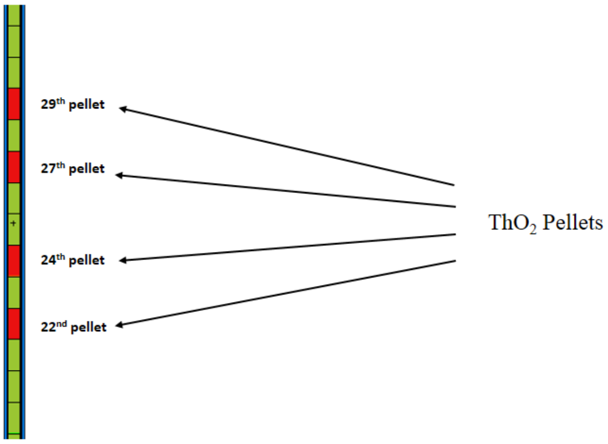

Figure 5. ThO$_2$ pellets placed middle of the rod.

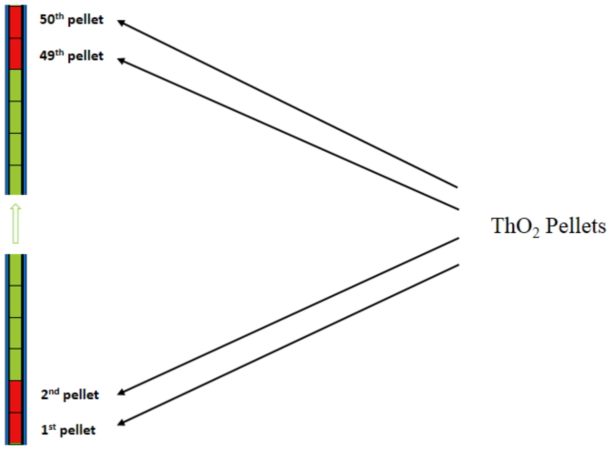

Figure 6. ThO$_2$ pellets placed top and bottom of the rod.

Table 1. MCNP simulation cases

Cases	Enrichment (wt.%)	Figure Number
^{235}U enriched pellets only	2.0	Figure 7
	2.5	Figure 8
	3.0	Figure 9
	3.5	Figure 10
	4.0	Figure 11
	4.5	Figure 12
	5.0	Figure 13
4 ThO_2 pellets are placed middle of the fuel rod	2.0	Figure 14
	2.5	Figure 15
	3.0	Figure 16
	3.5	Figure 17
	4.0	Figure 18
	4.5	Figure 19
	5.0	Figure 20
4 ThO_2 pellets are placed top and bottom side of the rod	2.0	Figure 21
	2.5	Figure 22
	3.0	Figure 23
	3.5	Figure 24
	4.0	Figure 25
	4.5	Figure 26
	5.0	Figure 27

the axially varying pellet distribution in the fuel pin. Burnup steps are prepared for MCNP inputs as 0, 0.52, 2.62, 7.87, 18.37, 34.11 GWd/MTU

For axial variation in pellet distribution, firstly, 2 cm pellets are filled with UO_2 with different enrichment ratios to take them as reference values. 4 ThO_2 pellets are placed middle of the rod, and, top and bottom of the rod as shown in Figure 5 and Figure 6, respectively.

4 Results

In order to observe the effects of thorium insertion in a fuel rod, the calculations performed for different pitch to diameter (P/D) ratios and three set of MCNP simulation cases summarized in Table 1 are prepared. In the first case, the calculations were performed for a pin reference filled with different ^{235}U enrichment levels. Change in reactivity with burnup for different P/D ratios, ^{235}U Enriched Rod (Reference Value), are shown in Figures 7-13.

In another case, 4 ThO_2 pellets are placed in the middle of the rod as shown in the Figure 5. For this case, the change in reactivity with burnup for different P/D ratios are present in Figures 14-20.

At the final case, 4 ThO_2 pellets are placed at the top and bottom side of the rod shown in Figure 6. Figures 21-27 show the reactivity change with changing burnup for different P/D ratios.

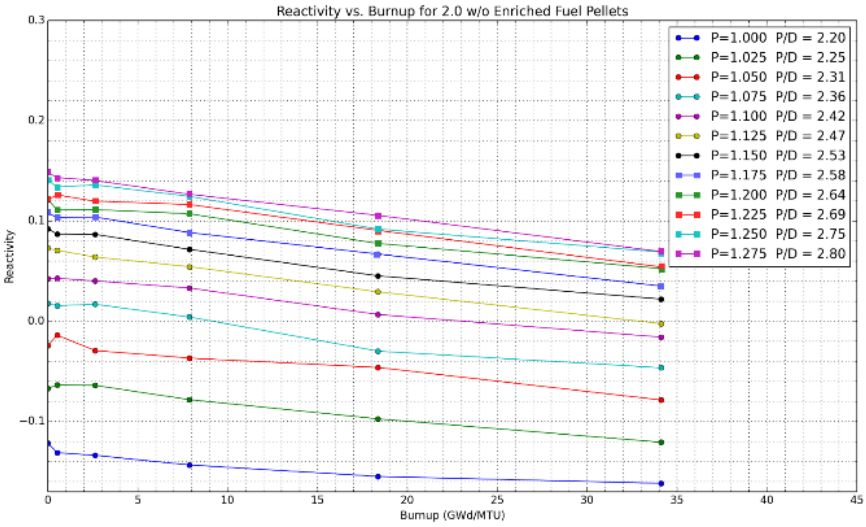

Figure 7. Burnup vs. reactivity values for 2.0 wt.% enrichment.

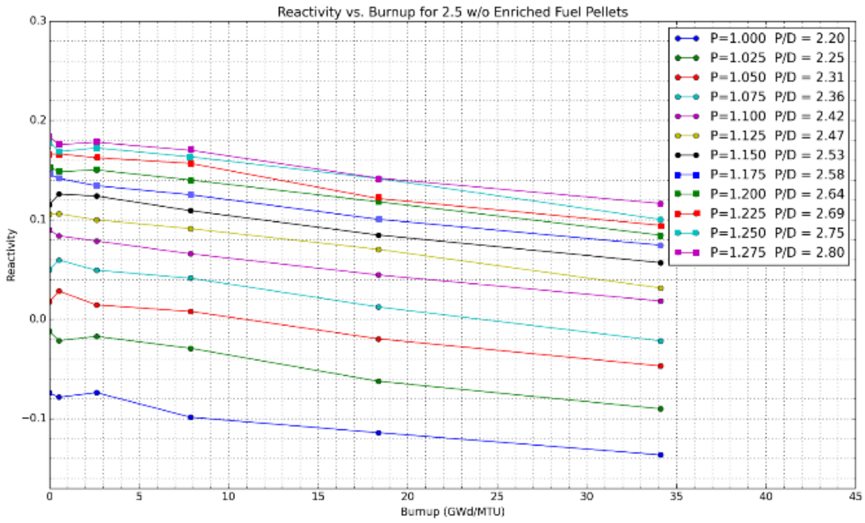

Figure 8. Burnup vs. reactivity values for 2.5 wt.% enrichment.

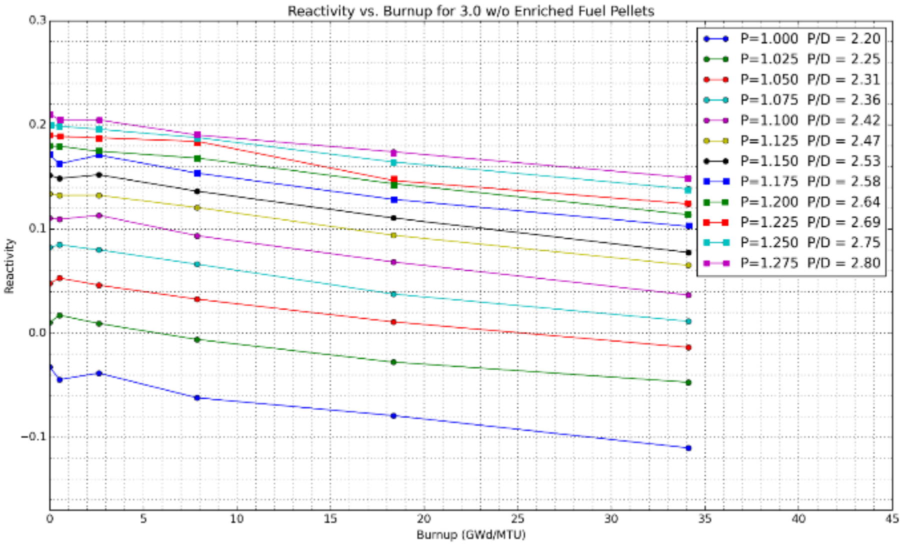

Figure 9. Burnup vs. reactivity values for 3.0 wt.% enrichment.

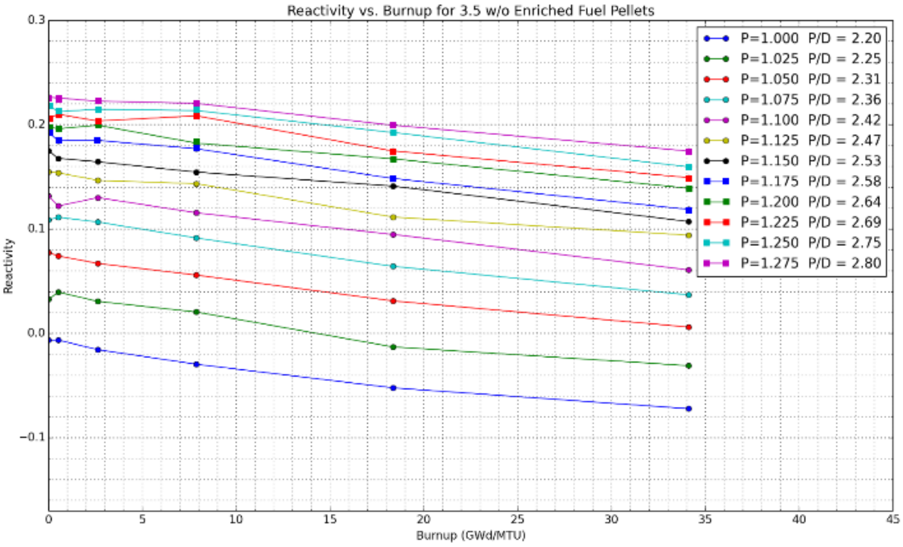

Figure 10. Burnup vs. reactivity values for 3.5 wt.% enrichment.

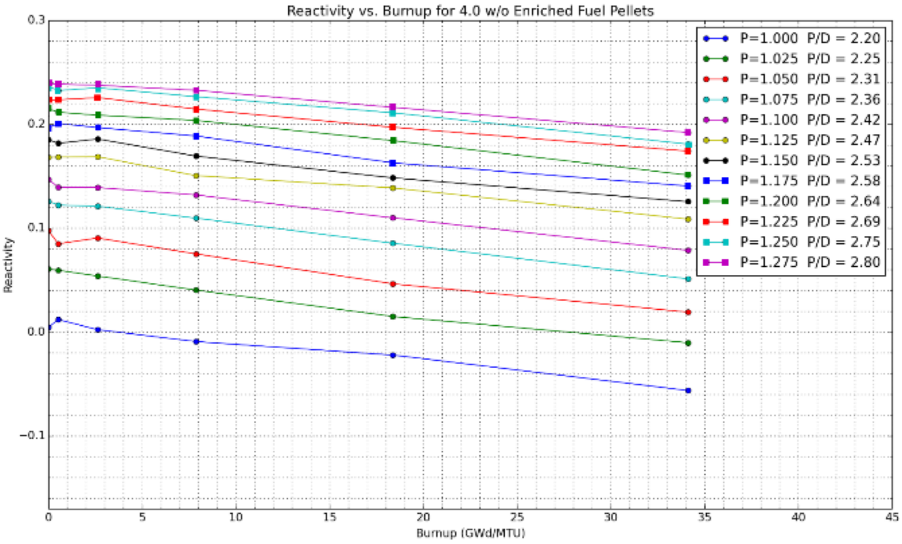

Figure 11. Burnup vs. reactivity values for 4.0 wt.% enrichment.

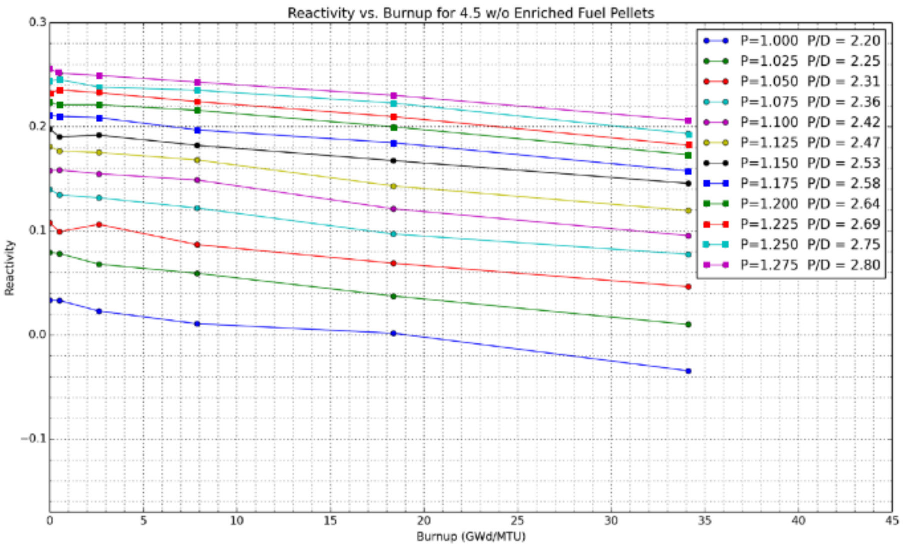

Figure 12. Burnup vs. reactivity values for 4.5 wt.% enrichment.

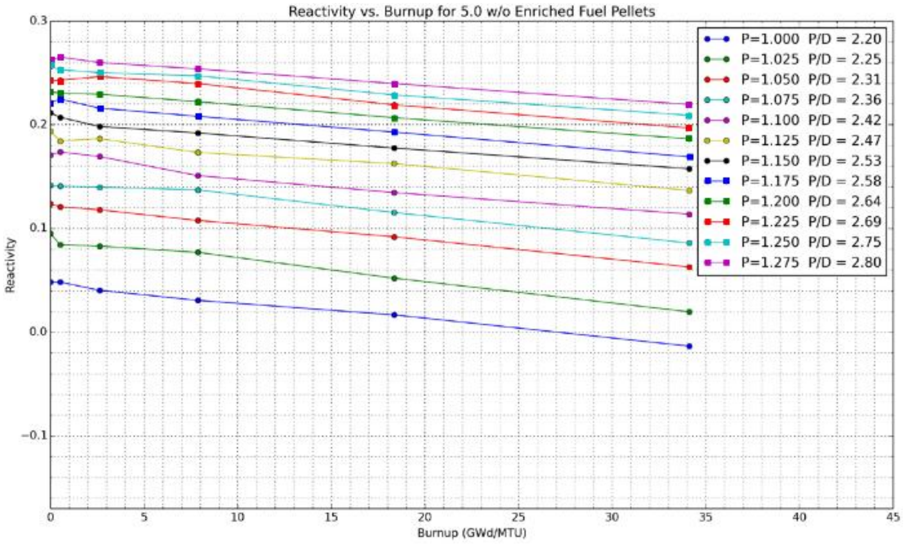

Figure 13. Burnup vs. reactivity values for 5.0 wt.% enrichment.

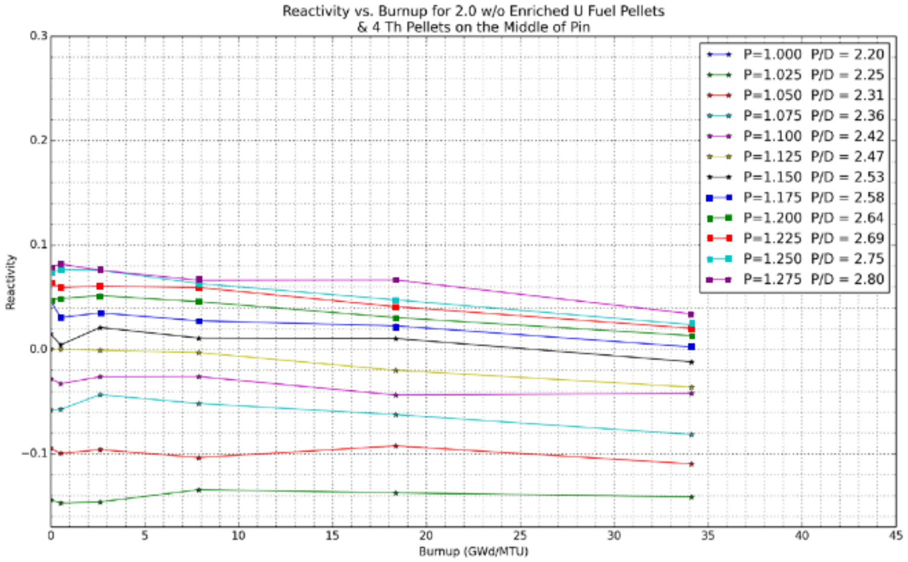

Figure 14. Burnup vs. reactivity values for 2.0 wt.% enrichment and 4 Thorium pellets placed middle of the rod.

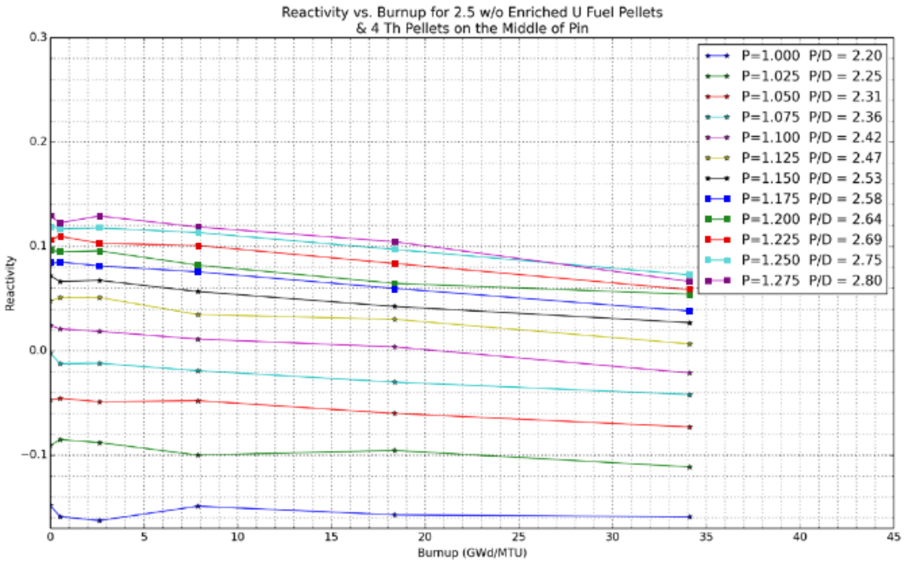

Figure 15. Burnup vs. reactivity values for 2.5 wt.% enrichment and 4 Thorium pellets placed middle of the rod.

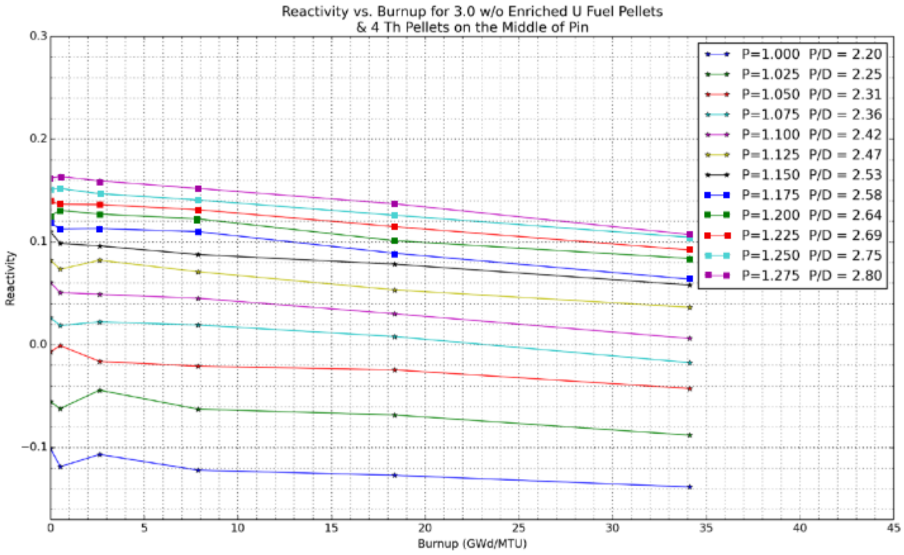

Figure 16. Burnup vs. reactivity values for 3.0 wt.% enrichment and 4 Thorium pellets placed middle of the rod.

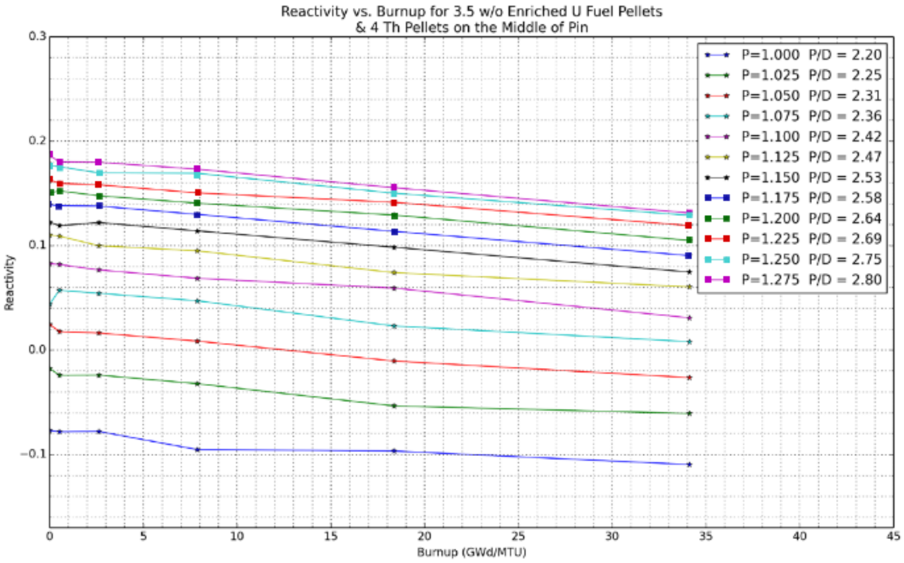

Figure 17. Burnup vs. reactivity values for 3.5 wt.% enrichment and 4 Thorium pellets placed middle of the rod.

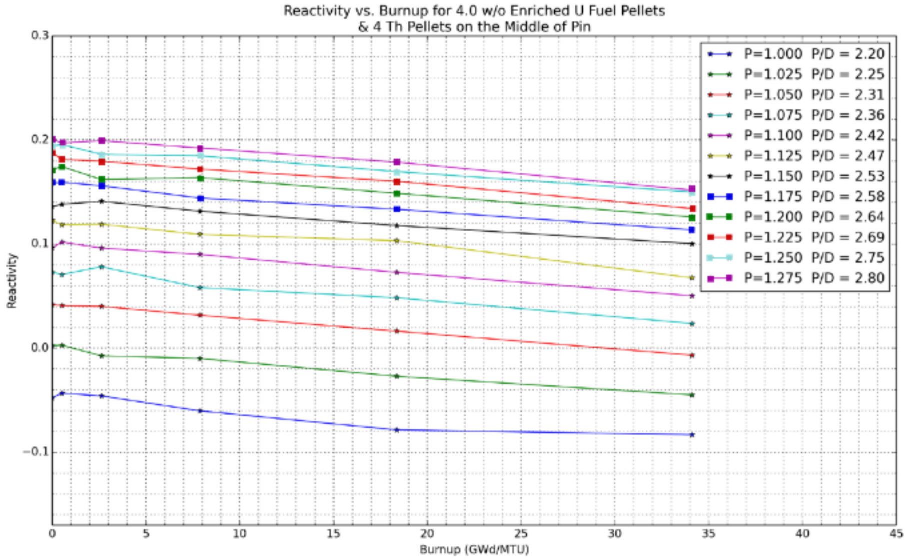

Figure 18. Burnup vs. reactivity values for 4.0 wt.% enrichment and 4 Thorium pellets placed middle of the rod.

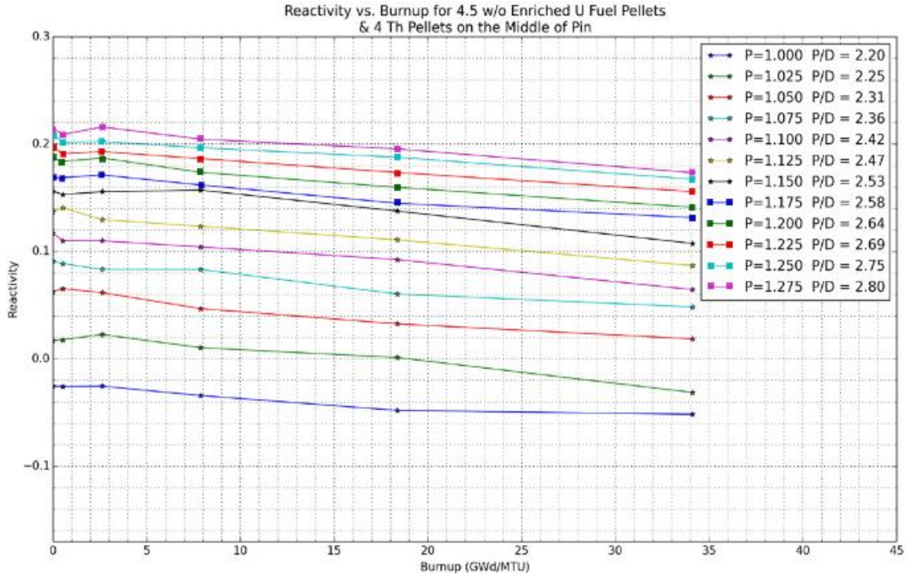

Figure 19. Burnup vs. reactivity values for 4.5 wt.% enrichment and 4 Thorium pellets placed middle of the rod.

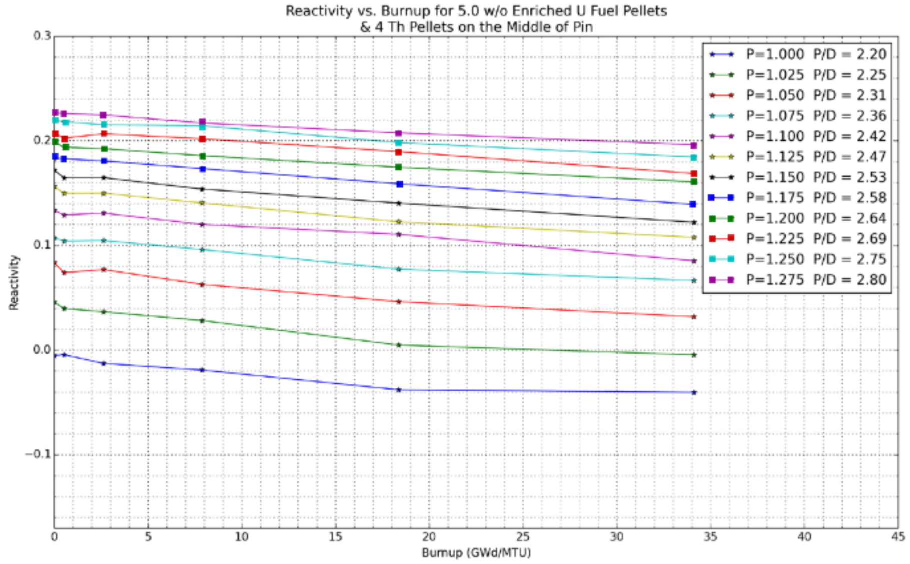

Figure 20. Burnup vs. reactivity values for 5.0 wt.% enrichment and 4 Thorium pellets placed middle of the rod.

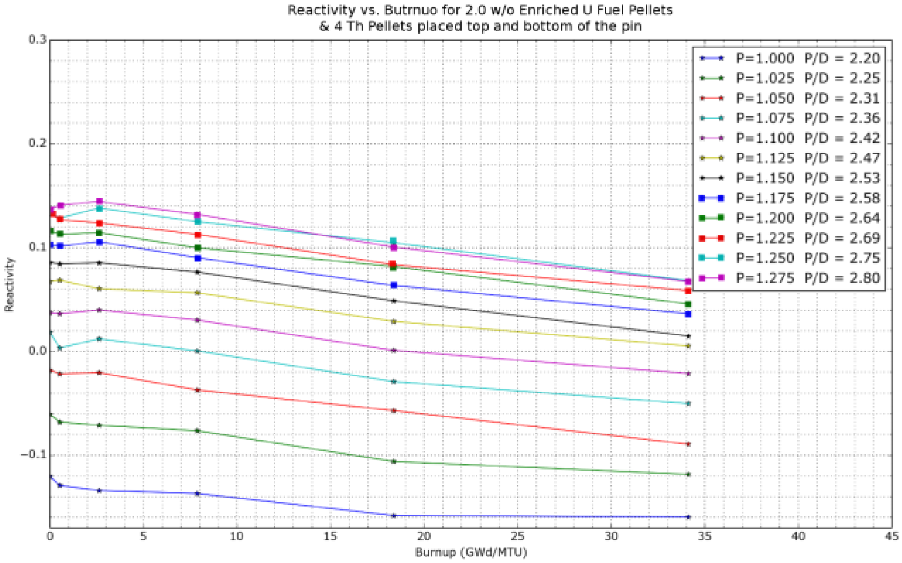

Figure 21. Burnup vs. reactivity values for 2.0 wt.% enrichment and 4 Thorium pellets placed top and bottom of the rod.

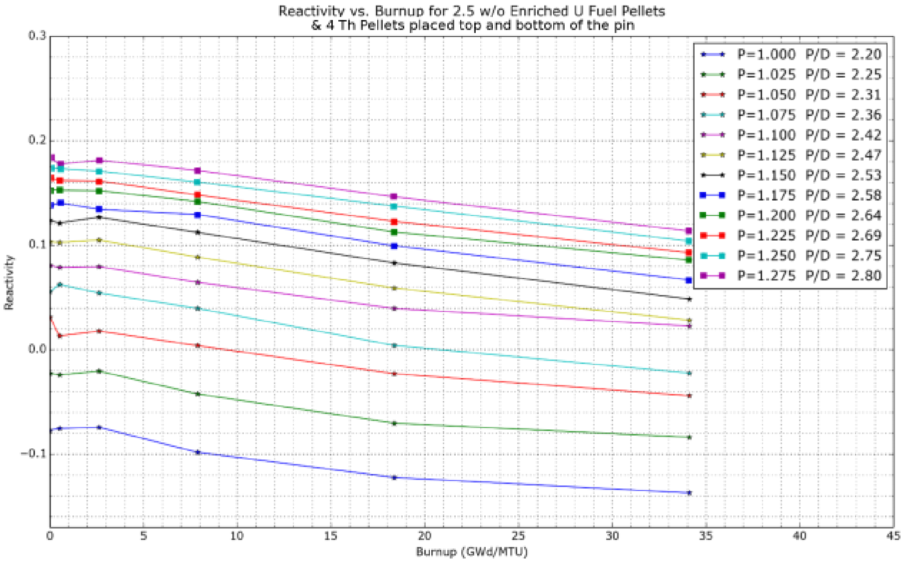

Figure 22. Burnup vs. reactivity values for 2.5 wt.% enrichment and 4 Thorium pellets placed top and bottom of the rod.

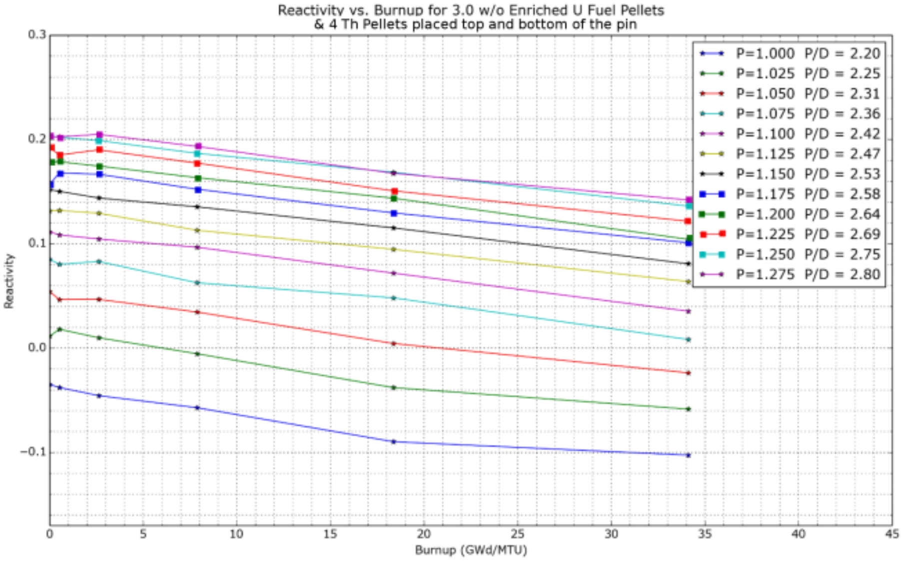

Figure 23. Burnup vs. reactivity values for 3.0 wt.% enrichment and 4 Thorium pellets placed top and bottom of the rod.

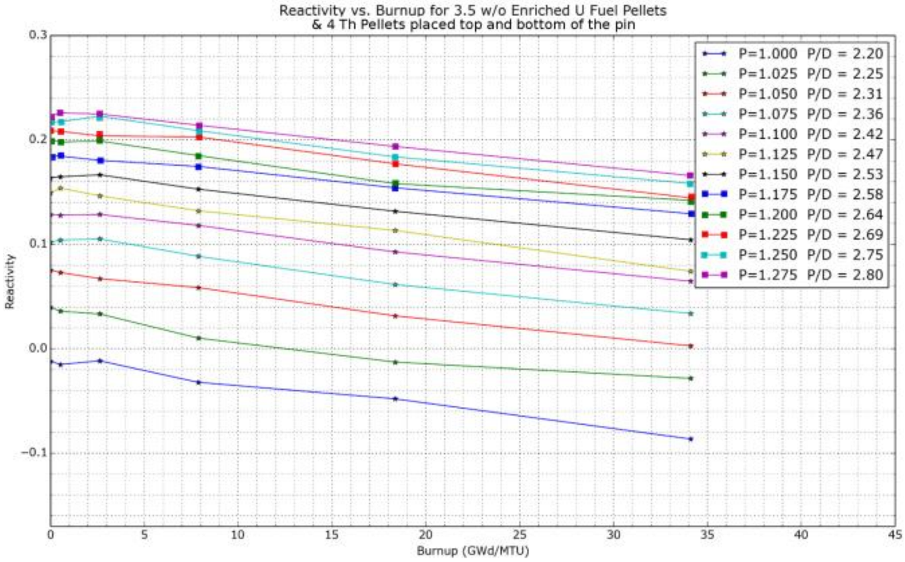

Figure 24. Burnup vs. reactivity values for 3.5 wt.% enrichment and 4 Thorium pellets placed top and bottom of the rod.

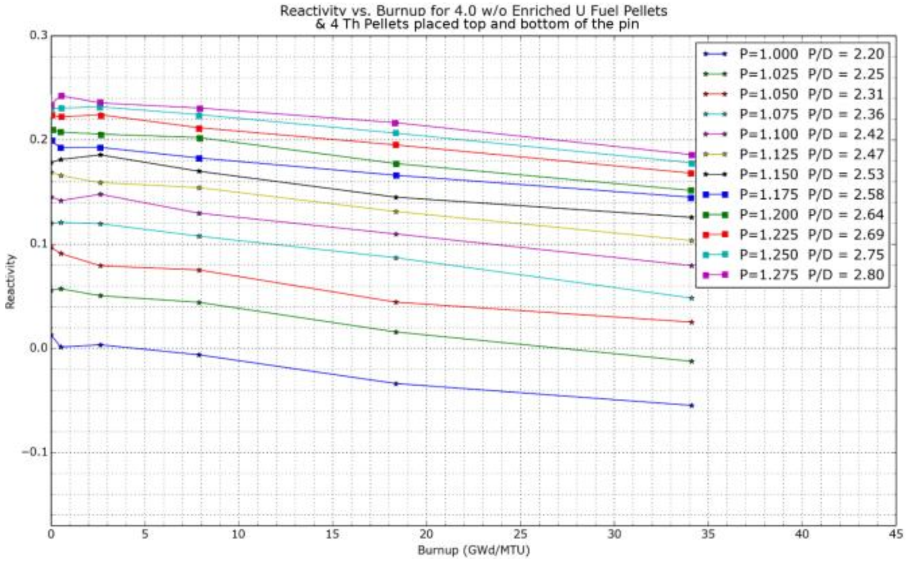

Figure 25. Burnup vs. reactivity values for 4.0 wt.% enrichment and 4 Thorium pellets placed top and bottom of the rod.

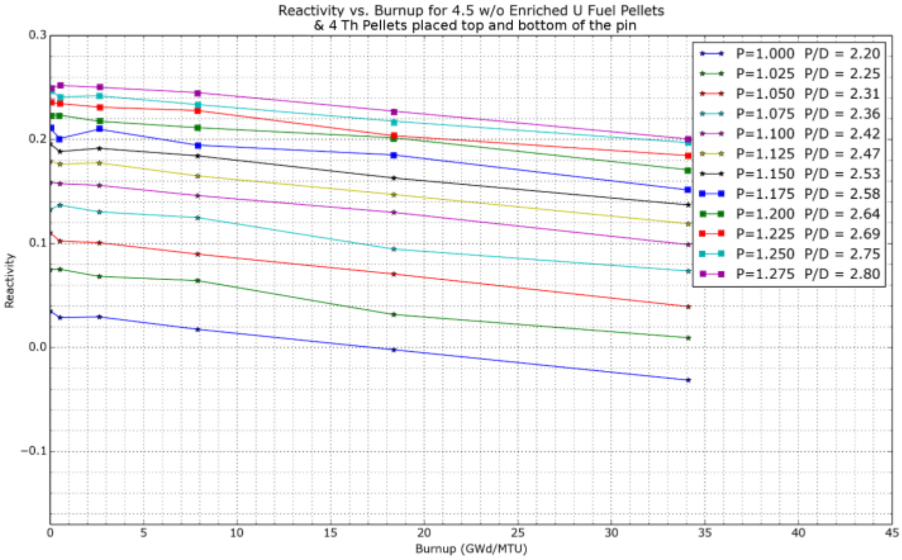

Figure 26. Burnup vs. reactivity values for 4.5 wt.% enrichment and 4 Thorium pellets placed top and bottom of the rod.

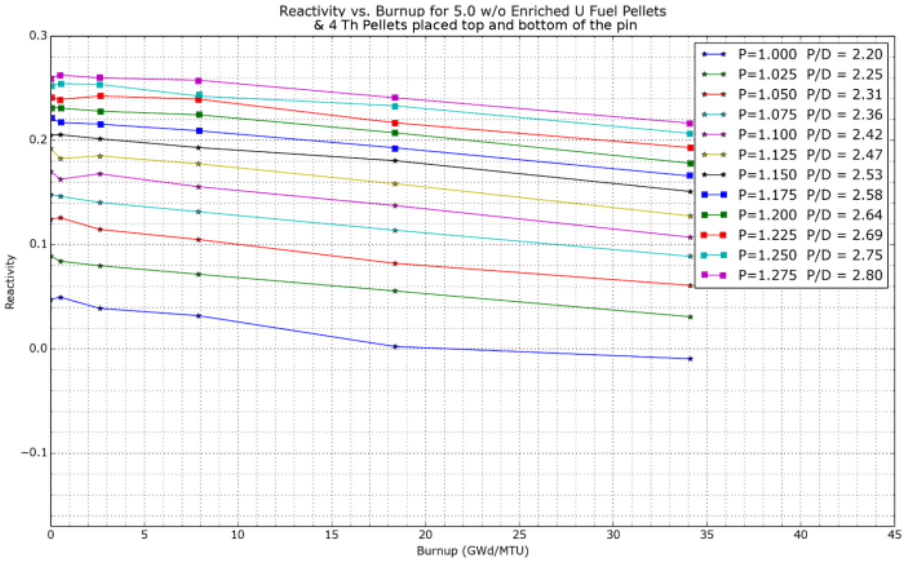

Figure 27. Burnup vs. reactivity values for 5.0 wt.% enrichment and 4 Thorium pellets placed top and bottom of the rod.

5 Conclusion

The criticality and burnup calculations were performing by using MCNP6.1.1 code system and its CINDER burnup module with new cross-section sets generated by NJOY99 for fuel pins including ThO_2 pellets. The calculations were performed for the pins pellet-by-pellet and 4 ThO_2 pellets were inserted at two different locations along the pin.

As it can be seen in the figures in the results, the decrease in pincell reactivity of thorium pellets placed in the middle is big. Since 4 ThO_2 pellets (extra absorber) are inserted into high flux location. Change in the pincell reactivity of thorium pellets placed in top and bottom results are very good for nearly all enrichment values. The reactivity changes are not significant. ^{233}U conversion is obtained in the ThO_2 pellets but the results are not enough for our breeding target.

As a future works, a new configuration set will be prepared with small burnup steps, in order to observe reactivity changes more precisely and to catch maximization of ^{232}Th-^{233}U conversion. The assembly based thorium added fuel cycles will be modelled to performing calculations for assemblies with varying rod size.

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