

# NEUTRONICS CHARACTERIZATIONS OF THE DUPLEX TRISO THORIUM FUEL ASSEMBLY BLOCKS USING MCNPX CODE

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## ABSTRACT

The  $UO_2$  seed and  $ThO_2$  blanket in the duplex fuel pellet were originally designed to increase the breeding rate of fissile materials in light water breeder reactors. In this configuration, most of the fission reactions occur in the seed portion, resulting in high temperature of the seed region. As such, duplex fuel pellet could possibly be advantageous for an application in a high-temperature reactor (HTR). In light of this observation, the paper aims to investigate the potential of duplex fuel pellet with TRISO fuel at the fuel block level. Specifically, the block-level neutronics performance of the typical TRISO fuel was compared to that of the TRISO duplex fuel using the MCNPX simulations. For the TRISO duplex pellet, a variety of packing fractions and seed's  $^{235}U$  enrichment were also simulated. In addition, the duplex TRISO fuel block was also modeled and compared to the standard  $UO_2$  block, homogeneous  $(Th,U)O_2$  fuel block, and seed and blanket unit (SBU) fuel block. It was noted that the duplex TRISO fuel compact has a noticeable longer operational cycle length than the  $UO_2$  TRISO fuel compact – these TRISO duplex fuels' cycle length and burnup were found to be significantly affected by variations in its packing fraction and seed enrichment. In addition, the duplex-rod fuel block and the SBU model also have comparable neutronics properties, as well as the highest power peaking. The combined method, in which the blanket  $ThO_2$  rods in SBU were replaced with duplex rods, can be used to manage these high power peaking issue by up to 23% reduction but with a shorter cycle length than the all duplex rods and SBU model. Nonetheless, the combined duplex + S&B configuration still has a longer cycle length than the standard  $UO_2$  block and homogeneous  $(Th,U)O_2$  fuel block models. These findings demonstrate the advantages of the duplex TRISO fuel design as a major optimization strategy for the future development of a thorium-loaded HTR.

## ABSTRAK

Bijian  $UO_2$  dan selimut  $ThO_2$  dalam pelet bahan api dupleks pada asalnya direka untuk meningkatkan kadar pembiakan bahan mudah pecah dalam reaktor pembiakan air ringan. Dalam konfigurasi ini, kebanyakan tindak balas pembelahan berlaku dalam bahagian benih, mengakibatkan suhu tinggi kawasan benih. Oleh itu, pelet rasa dupleks mungkin berfaedah untuk aplikasi dalam reaktor suhu tinggi (HTR). Berdasarkan pemerhatian ini, kertas kerja ini bertujuan untuk menyiasat potensi pelet bahan api dupleks dengan bahan api TRISO pada tahap blok bahan api. Secara khususnya, prestasi neutronik tahap blok bahan api TRISO biasa dibandingkan dengan bahan api dupleks TRISO menggunakan simulasi MCNPX. Untuk pelet duplet TRISO, pelbagai pecahan pembungkusan dan pengayaan  $^{235}U$  benih juga telah

*disimulasikan. Selain itu, blok bahan api TRISO dupleks juga telah dimodelkan dan dibandingkan dengan blok  $UO_2$  standard, blok bahan api homogen  $(Th,U)O_2$  dan blok bahan api unit benih dan selimut (SBU). Telah diperhatikan bahawa padat bahan api TRISO dupleks mempunyai panjang kitaran operasi yang lebih ketara berbanding padat bahan api  $UO_2$  TRISO - panjang kitaran bahan api dupleks TRISO dan pembakaran didapati terjejas dengan ketara oleh variasi dalam pecahan pembungkusan dan pengayaan benih. Selain itu, blok bahan api berrod dupleks dan model SBU juga mempunyai sifat neutronik yang setanding, serta memuncak kuasa tertinggi. Kaedah gabungan, di mana rod  $ThO_2$  selimut dalam SBU digantikan dengan rod dupleks, boleh digunakan untuk menguruskan isu memuncak kuasa tinggi ini dengan pengurangan sehingga 23% tetapi dengan panjang kitaran yang lebih pendek daripada semua rod dupleks dan model SBU. Namun begitu, konfigurasi dupleks + S&B gabungan masih mempunyai panjang kitaran yang lebih panjang daripada blok  $UO_2$  standard dan model blok bahan api homogen  $(Th,U)O_2$ . Penemuan ini menunjukkan kelebihan reka bentuk bahan api TRISO dupleks sebagai strategi pengoptimuman utama untuk pembangunan masa depan HTR yang dimuatkan torium.*

**Keywords:** Thorium Reactor; High Temperature Reactor; Micro Modular Reactor; TRISO-Duplex, MCNPX

## INTRODUCTION

Thorium is one of the available nuclear fuels in a fission power plant, and was thought as a one possible solution to solve the natural uranium shortages in the event of rapid nuclear power expansion [1]–[3]. Thorium is a fertile element that produces fissile material  $^{233}U$  when it absorbs neutrons [4]–[7].  $^{232}Th$  has been studied since the development of nuclear reactors in the 1950s and 1970s [6]. In light water thorium reactors in the 1970s and 1980s, duplex pellets were used to boost the breeding rate of fissile materials [8]. The duplex pellet incorporates  $UO_2$  and  $ThO_2$  of different volumetric ratios which are located next to each other. When duplex pellets were used in a fuel assembly or core configuration instead of the traditional seed and blanket fuel rod arrangement, its core conversion ratio (CR) was higher, which helped extending the core cycle [9]. Furthermore, the use of mixed thorium and uranium or homogeneous  $(Th,U)O_2$  necessitates the use of high  $^{235}U$  enrichment and lengthy thorium fuel irradiation in the reactor [10]–[13].

However, in light water breeder reactors, the major disadvantage of the traditional duplex design is the power imbalance caused by differences in fissile mass distribution. This issue arises as a result of a decrease in heat transfer efficiency from seed to coolant due to the presence of two layers between them, the fuel cladding and a blanket layer. Even at the typical linear power density of current PWRs, most of the energy released from the fission reaction originated from the seed region, resulting in significantly higher temperatures in the inner  $UO_2$  region [8]. This possibly compromises the pellet's material integrity, as well as causing gaseous fission product build-up inside the duplex pellet's gap between the  $UO_2$  and  $ThO_2$  sections.

In contrast, TRISO fuel is used in high-temperature reactors (HTR), which is safer in terms of fission product retention, creep strength, shrinkage under irradiation, and irradiation performance [14], [15], as well as more suitable with a high burnup environment and capable of keeping its integrity at high temperatures [16]–[18], up to 1600°C [19]–[21]. The HTR employs a helium coolant and a graphite moderator with high energy conversion efficiency, as well as a well-known passive safety mechanism. In addition, HTR is a well-developed reactor technology with competitive costs for both the graphite core and the TRISO design [22]. The use of duplex pellet design in thorium loaded HTR is expected to produce better results than previous applications in light water breeder reactors or PWRs.

The adaptation of the duplex pellet design in HTR TRISO fuel does not require physical separation of the fuel compact, as opposed to the original duplex pellet's air gap (see Figure 1). The configuration of  $ThO_2$  and  $UO_2$  fuel TRISO particles in the inner and outer layers of the fuel compact within the same graphite matrix is all that

separates the two parts. Even though the duplex design appears promising, there has been little research into its application in an HTR reactor. As a result, it's a good opportunity to compare the neutronics of the duplex's TRISO fuel compact to the  $\text{UO}_2$  TRISO. Therefore, this research was conducted to investigate the behavior of the TRISO fuel compact design that adopts the duplex concept for the HTR application. Using the MCNPX simulation, the neutronics performance of normal TRISO fuel was compared to that of TRISO duplex fuel, including performance at the fuel block level. Several comparisons were made between the different packing fractions of the Duplex TRISO fuel design and the  $^{235}\text{U}$  enrichment of the seed. The standard  $\text{UO}_2$  block, homogeneous  $(\text{Th,U})\text{O}_2$  fuel block, and seed and blanket unit (SBU) fuel block were also modeled and compared to the Duplex TRISO fuel block. Such a comparative study of some of the major parameters of reactor physics can support further investigations.

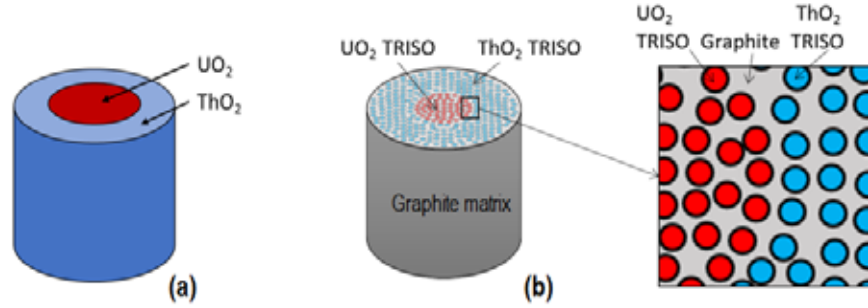


Figure 1. PWR Duplex fuel pellet (a) and the conceptual design of the duplex TRISO fuel compact (b)

## MATERIALS AND METHOD

The reference fuel and core parameter used in this study is based on the fuel design of the U-Battery micro modular HTR, which has already been widely published [23], [24], [33], [25]–[32]. Figure 2 shows the developed MCNPX model for the fuel and core design. The radius of the fuel particle and the radius of the fuel compact are 0.25 mm and 0.6225 cm, respectively. The TRISO particles are embedded in the fuel compacts, which are typical of prismatic HTR fuel design. They're cylinder-shaped and made up of TRISO and graphite matrix. The amount of fuel corresponds to a packing fraction of 30%, which is calculated as the ratio of total fuel particles volume to fuel compact volume.

The fuel block measures 36 cm in width and 80 cm in height. There are 216 fuel channels filled with fuel compacts, 108 coolant channels, and 15 TRISO fuel compacts with either  $\text{UO}_2$  or  $\text{ThO}_2$  particle in each channel. The fuel and coolant channels each have a diameter of 1.27 cm and 1.88 cm. Through this whole paper, the fuel channel is referred to as a fuel rod. The U-battery core (1.7 m in diameter) is made up of six columns of fuel blocks, with four fuel blocks arranged axially in each column. The central graphite column serves as a reflector, and the side reflectors are also made of graphite. The total core power is 10 MWth, and all calculations in this work are based on average power per fuel block and per fuel rod [35].

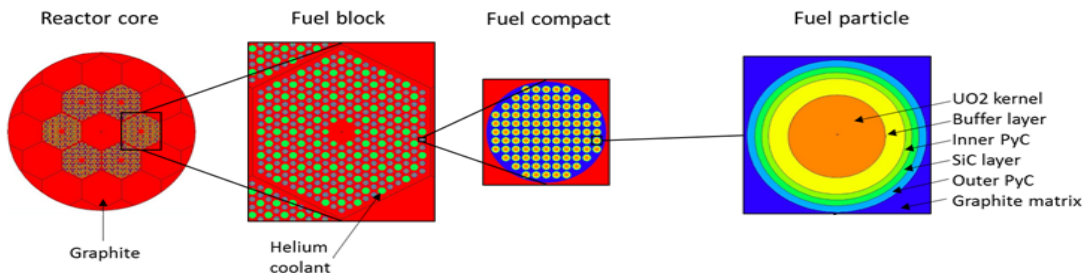


Figure 2. MCNPX model of reference core design fuel block fuel compact and the fuel particle

The Monte Carlo code MCNPX 2.7 was used to perform all calculations. This program is used to simulate steady-state reactions using the ENDF/B-VII.0 nuclear data library. It computes the neutron fluxes, reaction rates, and initial material eigenvalues in order to simulate the system's steady-state reactions. In order to calculate the depletion of isotopes and the new number densities of isotopic compositions of the fuel materials, the CINDER90 code was combined with MCNPX 2.7, a radioactive material depletion and burnup code [4]. This code is regarded as one of the most advanced 3D neutronic design tools, and it has been widely used to simulate and analyze HTR core and fuel burnup using a detailed or simplified geometry model. It can also simulate the random distribution of TRISO particles in an HTR fuel compact [34]–[37].

Figure 4 depicts the MCNPX duplex and TRISO reference fuel cell simulation models. The hexagonal graphite lattice surrounding the fuel rod is included in the fuel cell models. The  $\text{UO}_2$  seed TRISO particles are concentrated in the inner region of the TRISO duplex fuel rod, while the  $\text{ThO}_2$  TRISO particles form a blanket that fills the outer layer. The volume percentages between the inner ( $\text{UO}_2$ ) and outer ( $\text{ThO}_2$ ) regions were calculated using the  $\text{UO}_2$ : $\text{ThO}_2$  ratios of 25:75, 30:70, and 35:65, as recommended in previous research [8], [38]. In this study, the volume percentages of 30:70 were used.

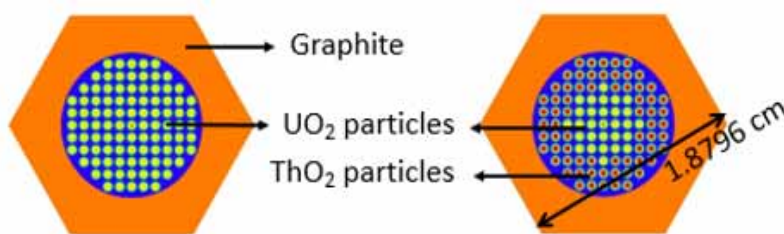


Figure 3. MCNPX reference (left) and Duplex TRISO (right) fuel cell model for analysis and comparisons

## RESULTS AND DISCUSSION

Figure 4 depicts three important burnup-related parameters: the evolution of the fissile material, the fissile inventory ratio (FIR), and the infinite multiplication factor ( $k_{inf}$ ) for both the  $\text{UO}_2$  TRISO and Duplex TRISO fuel compacts. The amount of energy produced by Gigawatt-day (GWd) per metric ton of heavy metal (MTHM) from the initial mass of the fuel is referred to as fuel burnup. To reduce nuclear waste and improve the plant's economics, a higher fuel burnup and a longer core cycle length were sought [39]. Both models have roughly the same  $^{235}\text{U}$  depletion and newly bred fissile buildup. The difference is in the type of fissile material, with  $^{239}\text{Pu}$  being the dominant fissile buildup in the  $\text{UO}_2$  TRISO fuel compact and  $^{233}\text{U}$  being the dominant fissile buildup in the Duplex TRISO fuel compact (in Figure 4(a) and Figure 4(b)). This is clearly due to the difference in  $^{238}\text{U}$  and  $^{232}\text{Th}$  content in both models. FIR comparison as shown Figure 4 (c) is a critical analysis for evaluating the conversion performance of fertile to fissile elements: calculated as a ratio of instantaneous to initial fissile nuclide inventory [40], [41].

The higher FIR in the reference fuel is clearly due to the slightly faster combined build-up of  $^{239}\text{Pu}$  and  $^{241}\text{Pu}$  in the reference fuel versus  $^{233}\text{U}$  build-up in the Duplex fuel. Nonetheless, as illustrated in Figure 4(d), the achievable exit burnup of the Duplex fuel compact is approximately 2.5 times that of the  $\text{UO}_2$  TRISO fuel compact. Even with the same initial fissile loading, the  $k_{inf}$  calculation shows that the Duplex TRISO fuel compact could maintain criticality of up to approximately 40 GWd/MTHM compared to only 13 GWd/MTHM for the  $\text{UO}_2$  TRISO fuel compact.

It should be noted that the Duplex TRISO fuel compact has the potential for lower plutonium buildup and higher burnup based on the results presented above. It was based on a packing fraction of 30%. Figure 5 shows an assessment of the Duplex fuel's achievable burnup at various packing fractions and seed enrichments. Burnup calculations were performed for a single fuel rod with a packing fraction of 20%, then for 25, 30, 35, and 40%. For each packing fraction case, there are four models, each with 12.5, 15, 17.5, and 20 wt%  $^{235}\text{U}/\text{U}$ . Obviously, a fuel model with a lower packing fraction has a higher moderator to fuel ratio, which contributes to a longer cycle

length and higher burnup. Furthermore, as enrichment increases, the model's  $k_{inf}$  value increases. When compared to the lower packing fraction model, the higher packing fraction fuel model requires more enrichment to achieve the same cycle length.

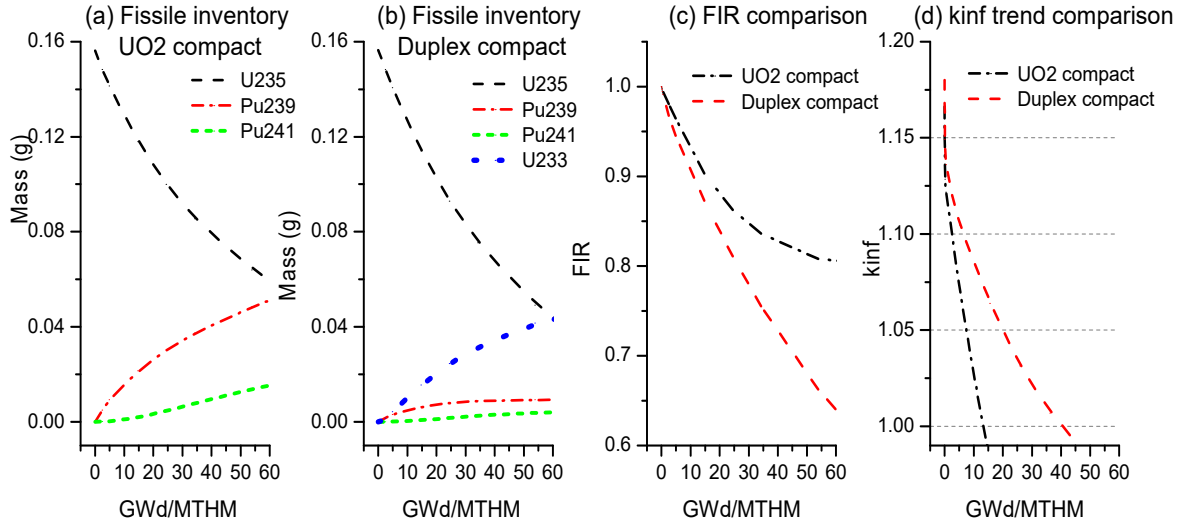


Figure 4. Fissile inventory for the reference UO<sub>2</sub> TRISO (a) and Duplex TRISO fuel compact, FIR (c) and the  $k_{inf}$  trend (d) comparison

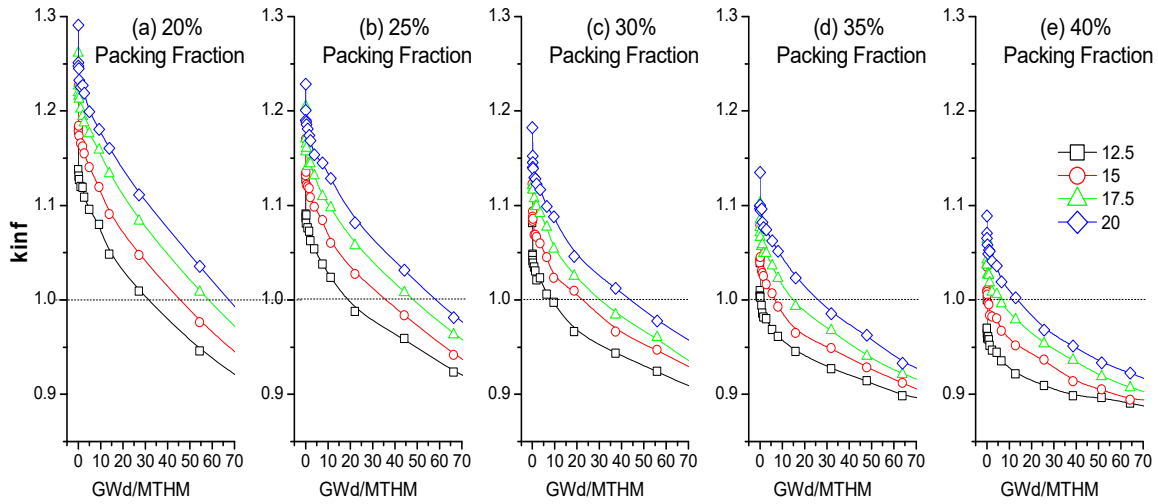


Figure 5.  $k_{inf}$  vs burnup for Duplex rods with different packing fractions and seed enrichment

Nonetheless, as shown in Figure 6, the lower the packing fraction and higher the seed enrichment, the lower the <sup>233</sup>U production, and vice versa, until approximately 60 GWd/MTHM is reached. At this burnup value and higher, the trend gradually shifts to the opposite, with higher enrichment resulting in higher <sup>233</sup>U buildup. The same buildup trend was seen for the <sup>239</sup>Pu buildup, with higher packing fractions (higher heavy metal mass) exhibiting greater plutonium buildup. <sup>239</sup>Pu buildup increases as seed enrichment increases. Figure 7 depicts the buildup of <sup>239</sup>Pu at various packing fractions and enrichments.

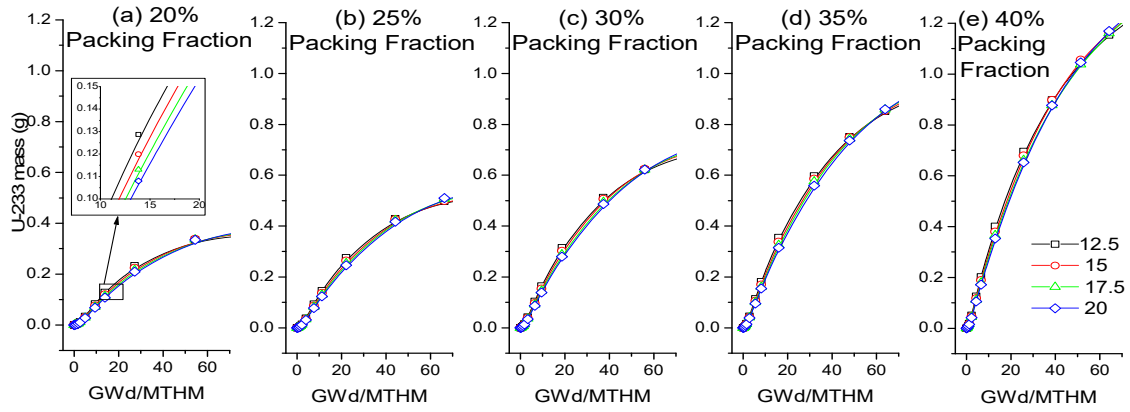


Figure 6.  $^{233}\text{U}$  buildup at various packing fractions and enrichment levels

As previously shown in Figure 5, the higher the heavy metal loading (the higher the packing fraction), the lower the  $k_{inf}$  value throughout the entire burnup period. The accumulation of parasitic actinides, including some plutonium isotopes, as well as the accumulation of  $^{233}\text{Pa}$ , a known strong neutron absorber, were responsible for this. The  $^{233}\text{Pa}$  would be lost through decay (to become  $^{233}\text{U}$ ) and neutron capture and it appears to reach equilibrium at the same mass, somewhere between 0.048 g and 0.05 g, regardless of packing fraction or enrichment. Figure 8 depicts this by extending the burnup data up to 160 GWd/MTHM. Despite having a longer cycle length and higher burnup than the higher packing fraction Duplex TRISO fuel rod model, the latter has the highest  $^{233}\text{U}$  accumulation. In a fuel block or core level configuration optimization, both conditions would play distinct roles and provide distinct benefits. Although it is beyond the scope of this paper to discuss the optimal fuel block or core design with Duplex fuel, the following section provides a preliminary analysis to demonstrate its performance at the fuel block design level.

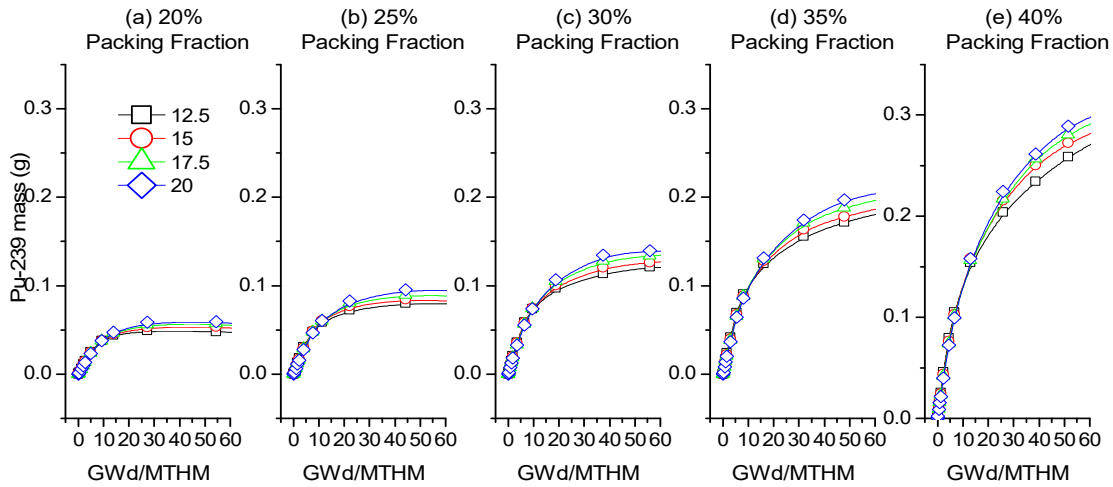


Figure 7.  $^{239}\text{Pu}$  buildup at various packing fractions and enrichment levels

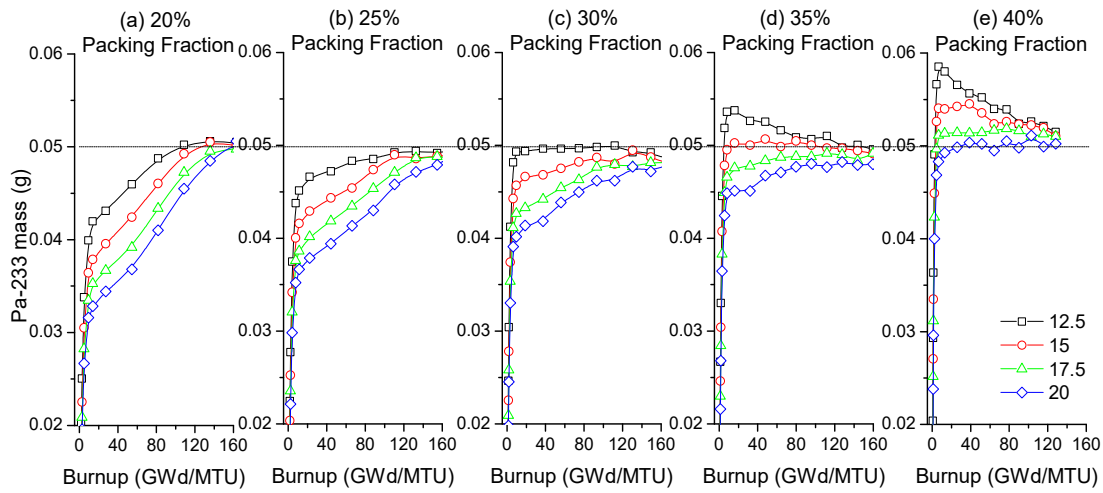


Figure 8. <sup>233</sup>Pa buildup at various packing fractions and enrichment levels

The Duplex TRISO fuel concept could still produce higher power density in the seed from the perspective of a single fuel rod. Duplex TRISO rods are planned to be used in a thorium seed-and-blanket fuel block or core as part of the optimization strategy. The use of a SBU block would also result in high-power peaking, particularly at the start of the cycle when the majority of the power comes from the fuel block's center. The SBU block configuration could be improved with the proposed TRISO duplex rod. Due to the lack of fissile material in the blanket region, which results in a high-power density in the seed of the SBU block, duplex rods may be used to replace blanket rods because they carry both fissile and blanket material. Since this distribution of <sup>235</sup>U fissile mass inside duplex pellets is now spread fairly within the blanket region, this optimized configuration should help flatten the neutron distribution across the fuel block. This, however, results in a lower thorium mass and thus a lower <sup>233</sup>U buildup. To demonstrate this statement, four fuel block models with different loading patterns are simulated, as shown in Figure 9, to compare neutron flux and power distribution, cycle length, and fissile inventory. The fuel block level analysis will use the same packing fraction as the original U-Battery reactor, which is 30%.

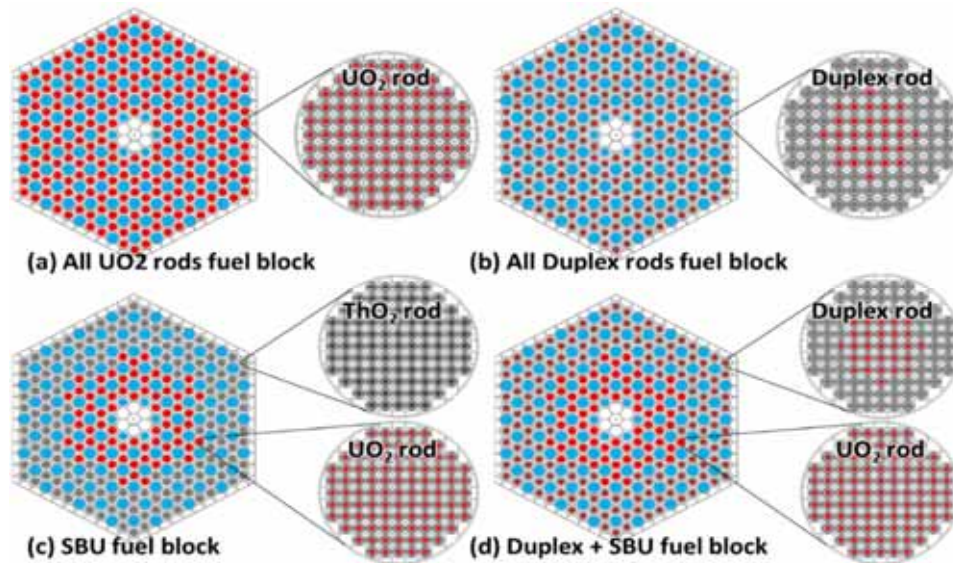


Figure 9. Loading pattern of fuel block models

Figure 10 compares the power, fast neutron, and thermal neutron distributions for the various fuel block models. The findings, as shown in Figure 10(b), reveal the challenges associated with the adaptation of the Duplex rod design, which is that the rate of fission reactions in the UO<sub>2</sub> region is more than threefolds that of the reference

model (in Figure 10(a)). The All Duplex rods fuel block has similar neutron flux and power distribution to the All UO<sub>2</sub> rod fuel block, but the power and fast neutron flux (both produced inside the fuel) are concentrated within a small region in the fuel rod. It has a maximum kernel power density of about 60 W/cm<sup>3</sup> (the All UO<sub>2</sub> rods fuel block has a kernel power density of only 20 W/cm<sup>3</sup>). The maximum kernel power density of the SBU fuel block is also three times that of the All UO<sub>2</sub> rods fuel block, with values of 65 W/cm<sup>3</sup> (Figure 10(c)). When compared to other fuel block models, it also has the most uneven neutron flux and power distribution. The integration with the duplex model produces a positive result as an optimization strategy for the SBU fuel block configuration. Figure 10(d) depicts the investigated Duplex + SBU fuel block design. The maximum kernel power density produced is approximately 50 W/cm<sup>3</sup>, which is 23% less than the SBU fuel block. Due to the obvious spread of the <sup>235</sup>U fissile mass distribution across the blanket region, the power and neutron flux distribution is more balanced after replacing the ThO<sub>2</sub> blanket rods with duplex fuel rods.

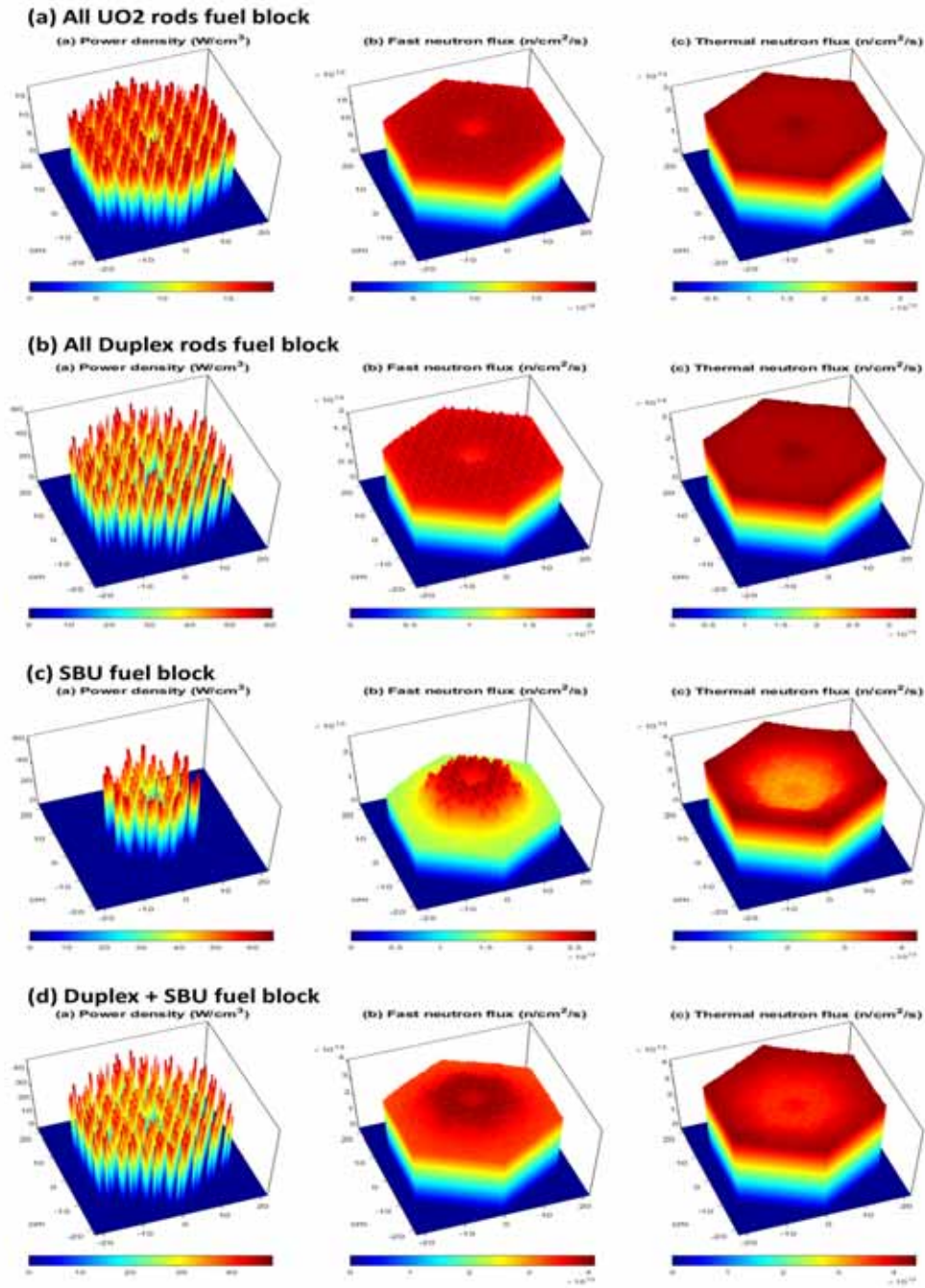


Figure 10. The distribution of neutron flux and power density for various fuel block models



It is discovered that as the thorium mass in the Duplex + SBU fuel block is reduced, the conversion rate outcome is not as good as in the SBU and All Duplex rods fuel blocks. Figure 11 shows that the Duplex + SBU fuel block has the lowest  $^{233}\text{U}$  buildup when compared to other thorium fuel blocks. As shown in Figure 12(a), it is assumed that the lower  $^{233}\text{U}$  build-up resulted in a 12 % lower burnup value when compared to the SBU block model. The SBU and the All Duplex rods fuel block models have an exit burnup of approximately 73 GWd/MTHM and 76 GWd/MTHM. The presence of  $\text{UO}_2$  in the blanket region, which increases neutron absorption competition with  $\text{ThO}_2$ , is assumed to reduce  $^{232}\text{Th}$  usage in the Duplex + SBU fuel block. Another fuel block model, the All  $(\text{Th,U})\text{O}_2$  rods fuel block, was also simulated. Due to the obvious even distribution of fissile material, the neutron flux and power distribution of this model were not included in Figure 10 because it is assumed that the results would be the same as all  $\text{UO}_2$  rod fuel block. However, its fissile inventory, as shown in Figure 11(e), is similar to that of All Duplex rods and SBU fuel blocks. The All  $\text{UO}_2$  rods fuel block and All  $(\text{Th,U})\text{O}_2$  rods fuel block were discovered to have the shortest cycle length, as shown in Figure 12(a), with criticality only being maintained up to 43 GWd/MTHM and 53 GWd/MTHM, respectively. Both, however, have a higher FIR value than the others.

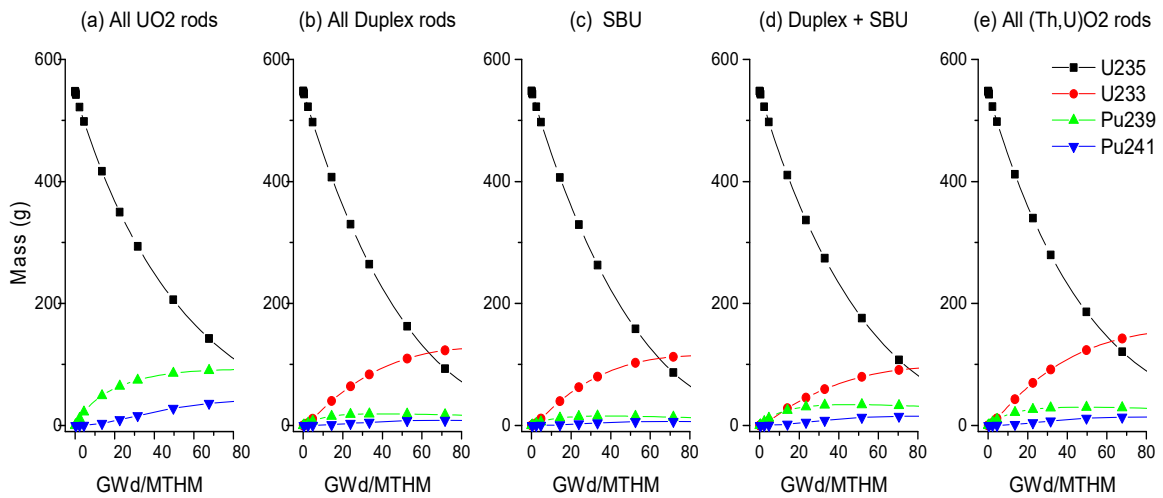


Figure 11. Fissile inventory comparison for various fuel block models

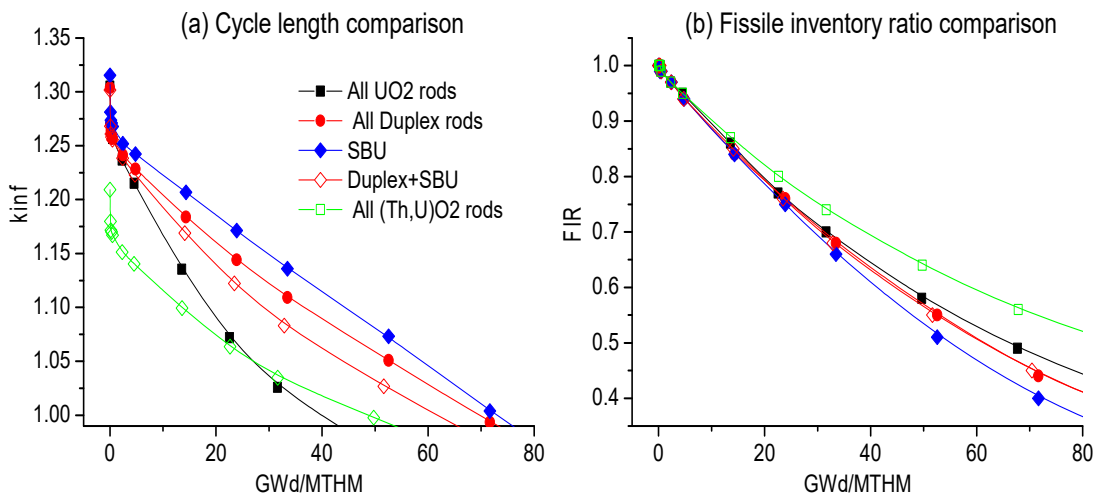


Figure 12. Cycle length and FIR comparison for various fuel block models

## CONCLUSIONS

The MCNPX simulation was used to compare the neutronic performance of normal TRISO fuel to that of TRISO duplex fuel, including performance at the fuel block level. The Duplex fuel has superior neutronic properties when compared to the reference UO<sub>2</sub> TRISO fuel compact, particularly the higher achievable fuel burnup. After that, the Duplex fuel composition was altered, and comparisons between different packing fractions and seed enrichment were made. Variations in packing fraction and seed enrichment were found to have a significant impact on cycle length and burnup, according to the findings. Duplex fuel with a lower packing fraction can achieve a longer cycle length, while fuel with a higher packing fraction can achieve a higher <sup>232</sup>Th to <sup>233</sup>U conversion. Higher packing fractions were found to result in more <sup>233</sup>Pa and plutonium buildup, lowering the kinf value.

The Duplex TRISO The standard UO<sub>2</sub> block, homogeneous (Th,U)O<sub>2</sub> fuel block, and SBU fuel block were also modeled and compared to the Duplex TRISO fuel block. When compared to the reference UO<sub>2</sub> block, thorium fuel blocks have a longer cycle length and higher burnup. Furthermore, the heterogeneous thorium fuel block models All Duplex rods, SBU, and Duplex + SBU could achieve higher fuel burnup than the homogeneous All (Th,U)O<sub>2</sub> rods fuel block. However, the heterogeneous thorium fuel blocks have the most unstable neutron flux and power distribution. Nonetheless, the combine method, which replaced the blanket ThO<sub>2</sub> rods in SBU with Duplex rods, was found to reduce the high power peak by up to 23% while having a shorter cycle length than all Duplex rods and the SBU model. Based on these findings, it is recommended that further research and design analysis be conducted on the use of the Duplex TRISO fuel in a thorium HTR. Overall, the results show that the Duplex TRISO fuel design can be used as part of an optimization strategy for the future development of a thorium-loaded HTR.

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