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Neutronic Assessment of High-Temperature Gas-Cooled Thorium Burner using Monte Carlo Calculation Method with Full Core Model

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Monte Carlo
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Yanma Analizi
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Graphical/Tabular Abstract (Grafik Özet)

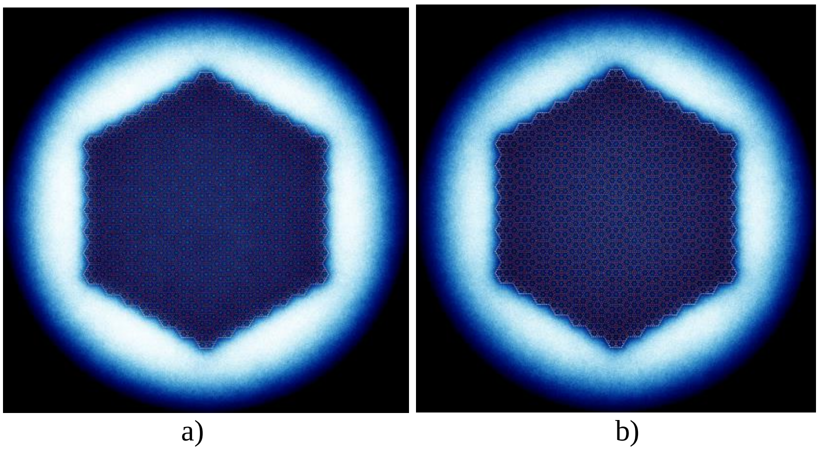

Figure A: *a) burning at the beginning / HTGR tam çekirdeğinde başlangıçta yanma, b) burning at the end of life of HTGR full core / işletim zamanı sonu yanma*

Highlights (Önemli noktalar)

- *3D heterogeneous reactor analysis / 3D heterojen reaktör analizi*
- *SiC cladding effect on reactivity / SiC kaplamanın reaktivite üzerindeki etkisi*

Aim (Amaç): *To examine the effect of SiC and ZrC compounds on the reactivity differences between 3D heterogeneous reactor analysis and semi-homogeneous reactor analysis. / SiC ve ZrC bileşiklerinin 3D heterojen reaktör analizi ve yarı homojen reaktör analizi arasındaki reaktivite farklılıkları üzerindeki etkisini incelemek.*

Orginality (Özgünlük): *3D heterogeneous reactor analysis, Analyze with SiC cladding. / 3D heterojen reaktör analizi, SiC kaplama ile analizi*

Results (Bulgular): *The burnup value has been computed as 189 GWd/ton and it was observed that the reactor operation time is up to 4500 days when the high-quality graphite used as a moderator. / Yakma değeri 189 GWd/ton olarak hesaplanmış ve moderatör olarak kaliteli grafit kullanıldığında reaktör çalışma süresinin 4500 güne kadar çıktığı gözlemlenmiştir.*

Conclusion (Sonuç): *SiC, which has smaller neutron absorption cross sections has a positive effect on reactivity compared to ZrC. / Daha küçük nötron absorpsiyon kesitlerine sahip olan SiC, ZrC'ye kıyasla reaktivite üzerinde olumlu bir etkiye sahiptir.*

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Neutronic Assessment of High-Temperature Gas-Cooled Thorium Burner using Monte Carlo Calculation Method with Full Core Model

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Abstract

In this study, the effective reactivity and burnup analyses have been performed for heterogeneous three-dimensional high-temperature gas-cooled thorium reactor (HTGR) which has 60 MWth full core geometry by using continuous-energy multi-purpose three-dimensional Monte Carlo particle transport Serpent code with ENDF/ B-VII data libraries. Nuclear fuel has been selected as 50 % ThO_2+50% RG-PuO_2. Firstly, effective reactivity for three different qualities of graphite for operation period have been determined. The effective reactivity showed better performance with increasing densities of graphite. Secondly, it has been also examined to ZrC and SiC cladding materials effect on the effective reactivity. It is observed that SiC has a positive effect on reactivity compared to ZrC. As a results, the full core life low-power thorium-burner HTGR have been calculated as up to ~4500 days depending on the graphite material whereas, the corresponding burnups came out to be ~ 189 GWd/ton, for end of life.

Monte Carlo Hesaplama Yöntemi Kullanılarak Yüksek Sıcaklıkta Gaz Soğutmalı Toryum Yakıcının Tüm Çekirdek Modeli ile Nötronik Değerlendirilmesi

Makale Bilgisi

Araştırma makalesi
Başvuru: 24/05/2023
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Anahtar Kelimeler

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Öz

Bu çalışmada, ENDF/ B-VII veri kütüphaneleriyle sürekli enerji çok amaçlı üç boyutlu Monte Carlo parçacık taşınım kodu SERPENT kullanılarak 60 MWth güce sahip reaktörün, tüm çekirdek geometriyle heterojen üç boyutlu yüksek sıcaklıklı gaz soğutmalı toryum reaktörü (HTGR) için etkin reaktivite ve yanma analizleri yapılmıştır. Nükleer yakıt %50 ThO_2+%50 RG-PuO_2 olarak seçilmiştir. İlk olarak, üç farklı kalitede grafit için işletme süresi boyunca etkin reaktivite belirlenmiştir. Elde edilen sonuçlara göre Etkin reaktivitenin, artan grafit yoğunluklarıyla daha iyi performans gösterdiği görülmüştür. İkinci olarak ZrC ve SiC kaplama malzemelerinin etkin reaktivite üzerindeki etkisi incelenmiştir. SiC'nin ZrC'ye kıyasla reaktivite üzerinde olumlu bir etkiye sahip olduğu görülmektedir. Sonuç olarak, düşük güçlü toryum yakıcı HTGR'nin tam çekirdek ömrü grafit malzemeye bağlı olarak ~4500 gün olarak hesaplanmış, son güne karşılık gelen yanma ise ~ 189 GWd/ton olarak çıkmıştır.

1. INTRODUCTION (GİRİŞ)

Nuclear wastes have been generated during the nuclear electricity generation of different countries for the last 50 years using nuclear energy, and the vast majority of these wastes are civilian plutonium stocks. Currently, reactor grade plutonium is estimated at around 1700 tonnes. Since there is a serious concern in the world about the misuse and radiotoxic release of this plutonium, which is obtained as nuclear waste, it is of interest to evaluate and reduce the plutonium stocks as nuclear fuel. For the management of plutonium, incineration is one of the alternative methods. However, if plutonium nuclear waste is used in the form of uranium/plutonium mixed oxide (MOX), second generation plutonium will be produced. Another alternative method is to burn plutonium with thorium fuel. Since thorium cannot be a used alone, plutonium must be used as fissile fuel material for the thorium fueled reactor [1]. Previous work has investigated the incineration of plutonium in CANDU reactors [2-4], Fixed bed nuclear reactor (FBNR) [5], high temperature pebble bed nuclear reactors (PBMR)[6] and high-temperature gas-cooled reactor (HTGR) [7-9] in combination with

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thorium extensively in detail. There is a large-scale study for III+ generation nuclear reactor around the world in the literature. One of these reactors is high temperature gas cooled nuclear reactor (HTGR). HTGR types of reactors could consider transition of VHTGR. In recent years, developments on low-power, high-temperature gas-cooled reactors (HTGR) have been a source of light in the development of nuclear energy. Low-capacity modular HTGRs is studied in the United States, Russia, Germany, France and Japan, which have well-developed nuclear energy programs, and further studies on the development of HTGR continue in Korea, China, South Africa and India [9-13]. HTGR type reactors which has different pellet sizes and fuel assemblies have been usually analysed by the reactor core cell method by I.V. Shamanin [8] by using neutronic computer codes of the MCU-5 series. Also, HTGR used in the calculations is based on a 78-channel fuel assembly by using neutronic computer codes of the MCU-5 series [9]. TRISO particle which has outer layer Ti_3SiC_2 clad as fuel inside fuel pellet which has SiC clad, was used in the geometry. SiC is a newer cladding material than ZrC in literature. In some studies, ZrC was used as a cladding material. In another study, ZrC and SiC materials were compared [14]. In addition, with the development of technology because of engineering studies, there has been a significant increase in thermal efficiency. The efficiency of gas turbines in HTGR is up to 50 percent as pointed by H. C. No. [15].

Looking at recent studies, research and development studies in reactors are mostly carried out in small modular reactors (SMR). According to the classification adopted by the International Atomic Energy Agency (IAEA); Small Reactors are reactors with installed electricity generation power of less than 300 MWe, Medium Reactors are reactors with installed electricity generation power between 300 and 700 MWe. The Small Modular Reactors class includes Integrated Pressure Water Reactors, Molten Salt Reactors, High Temperature Gas Cooled Reactors, Liquid Metal Cooled Reactors, and Solid State or Heat Pipe Reactors. SMRs contain innovative features in some of their designs. In some designs, coolant systems can use natural convection to eliminate pumps. Accordingly, Loss of Coolant Accidents (LOCA) are prevented [18]. They have negative temperature coefficients in the moderator and fuel. This situation keeps the fission reactions under control and causes the reaction to slow down when the temperature increases [19]. SMRs stand out because they are safe, cost effective and can produce clean energy. Small Modular Reactors stand out compared to Light Water Reactors due to their low investment costs and small size. These reactors are generally designed to serve military garrisons, desalinate, power generation, produce high-quality heat, deliver energy to places where the grid connection cannot reach, and be used in other industrial services. SMR designs may use light water or other refrigerants such as gas, liquid metal, or molten salt as the coolant. In addition to being portable, it also provides great advantages that they have fast installation.

Looking at recent studies of HTGRs, HOLOS reactor comes to the fore. HOLOS is a HTGR type reactor designed in accordance with the micro-reactor concept. HOLOS consists of four subcritical power modules. These modules combine to make the reactor critical. It can produce 22 MW of thermal energy. In the core, there are 151 hexagonal fuel assembly. Each of these assembly contains 19 fuel channels and 54 cooling Helium gas channels. Zirconium element is used as the envelope material on the outer part of the cooling channels. Similarly, to prevent the direct interaction of the reflective part of the reactor with the air, a layer of Zirconium was placed on the outer part of the reflector made of Beryllium. More information on the HOLOS reactor can be found in Stauff's study [20].

Finally, if we summarize HTGRs, Graphite is used as a moderator and Helium is used as a coolant in HTGRs. The main reason for using Helium as a coolant is that Helium is an inert gas and accordingly it does not react chemically with any substance. Also, Helium does not become radioactive when exposed to neutrons.

In this paper, unlike in the literature, the effect of the SiC and ZrC cladding materials on criticality in the HTGR have been performed of the heterogeneous 3D full core geometry. Neutronic calculations have been performed the Serpent code [16] which has a continuous-energy Monte Carlo reactor physics burnup calculation code with ENDF/ B-VII cross section, decay and fission libraries. In addition, the effects of the quality of the graphite used on the effective reactivity and amount of burning thorium has been compared with literature.

2. Methods & Calculations (Metot & Hesaplamalar)

The vertical and horizontal view of the low power HTGR obtained by using Serpent Monte Carlo nuclear code has been given in Figs. 1 and 2. There are 127 assemblies in the reactor. Each assembly consists of 78 hexagonal fuel channels and 7 coolant channels. Each fuel channel included 120 fuel pellets with SiC clad. Technical specifications of the simulated low power HTGR have been presented in the Table 1 [8-9]. In the calculations model which has 78-channels hexagonal assembly has been used. The hexagonal assembly has been shown in Fig.3. In this assembly, big bores are symbolized to helium channel and its radius are equal to 1.2 cm. Small bores are symbolized to fuel channel and its radius are equal to 0.6 cm. Flat to flat dimension of hexagonal assembly is equal to 20 cm. All technical details can be found in the I.V. Shamanin's studies [8-9].

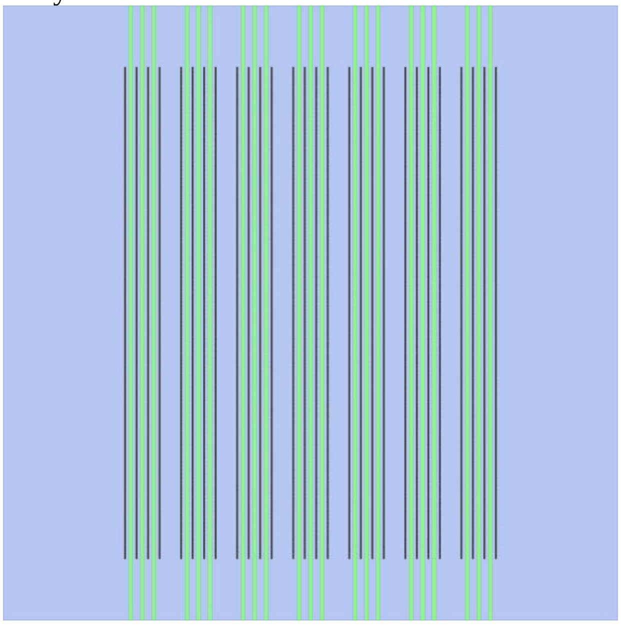


Fig. 1. Vertical Section of the HTGR full core model

(HTGR tam çekirdek modelinin dikey kesiti)

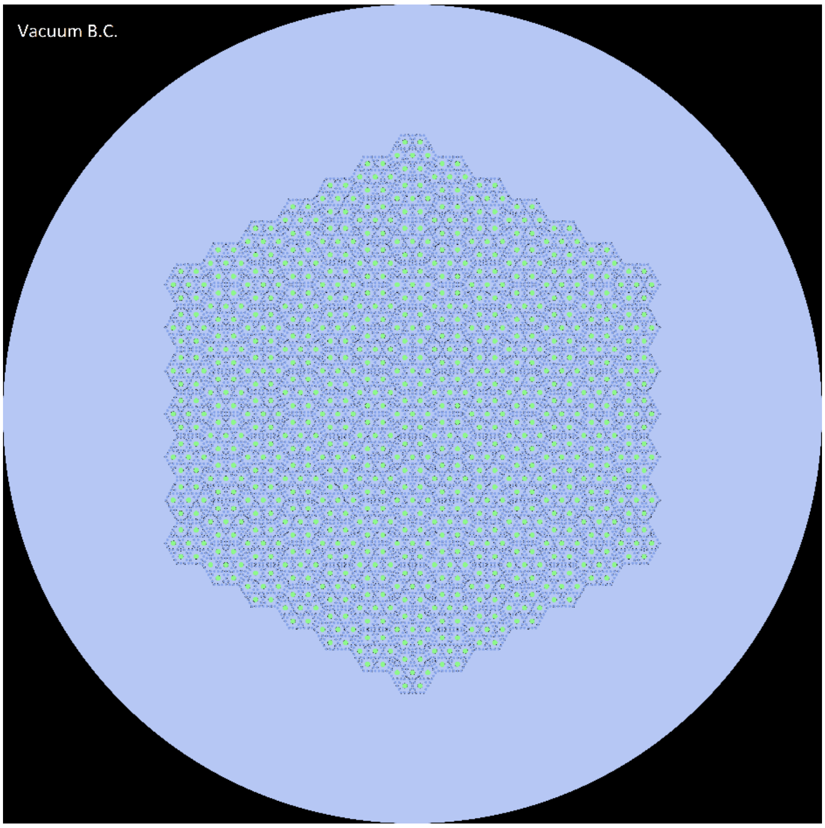


Fig. 2. Horizontal Section of the HTGR full core model

(HTGR tam çekirdek modelinin yatay kesiti)

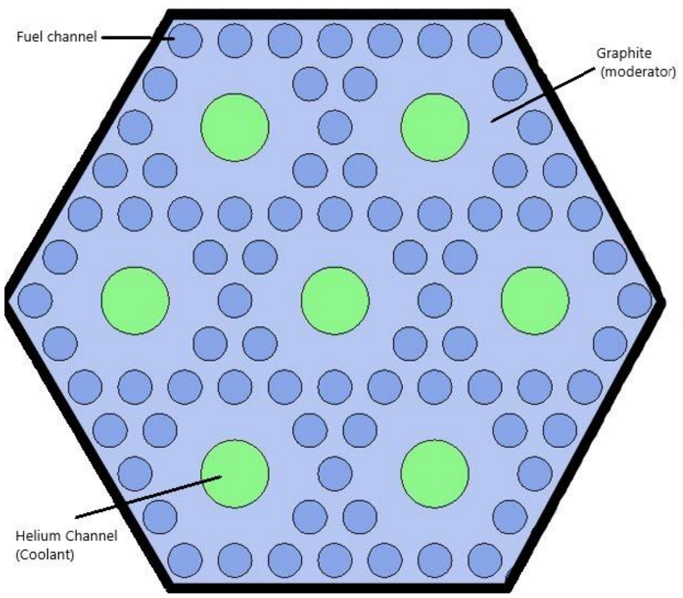


Fig. 3. Hexagonal bundle assembly view of the HTGR

(HTGR'nin Altıgen Yakıt Demeti Görünümü)

Table 1. Technical data of simulated core LPHTGR [8] (Simüle çekirdek LPHTGR'nin teknik verileri)

Specification	Value
Thermal power (MWth)	60
Efficiency factor (%)	up to 50
Height of core (m)	2.4
Height of core with reflector (m)	3.0
Core radius with reflector (m)	1.5011
Reflector thickness (m)	~0.20
Pellet diameter with clad (m)	0.0120
Pellet diameter (m)	0.0114
Height of pellet with clad (m)	0.020
Operating temperature (K)	1250

A pellet figure in which pebbles has been dispersed is given Fig. 4. The inside of the pellet consists of sintered graphite. The pebbles have been dispersed on the sintered graphite surface. The clad of the pellet is a thin SiC surface. In addition, ZrC has been used as a cladding material on its outer surface to examine its effect to reactivity.

The particles dispersed on the pellet have been given in Fig. 5. The materials used in the regions of this sphere are fuel, pyrolytic carbon and Ti_3SiC_2 respectively, starting from the center. A mixture of heavy grade Pu and Th was used as fuel. Fuel region in the pebble image consists of (Pu, Th)O_2. The isotope amount of Pu and Th are taken from the study made by Shamanin.[9] study. The fuel has produced with a ratio of 50 % ThO_2+50% RG-PuO_2. The density of the fuel is 10.4 g/cm^3. The isotope ratio of Pu has been given in Table-2

Table 2. Isotopic concentration data of Pu [9]. (Pu'nun izotopik yüzdelik verileri)

Pu isotopic composition	^{238}Pu (%)	^{239}Pu (%)	^{240}Pu (%)	^{241}Pu (%)	^{242}Pu (%)
Fraction	1.8	59	23	12.2	4

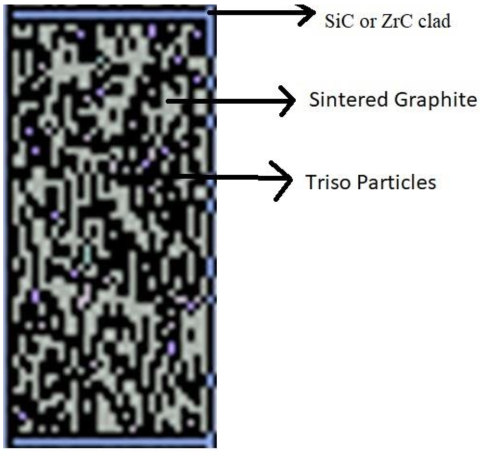


Fig. 4. Calculation fuel pellets model of fuel assembly

(Yakıt demetinde yakıt pelet modelinin hesaplanması)

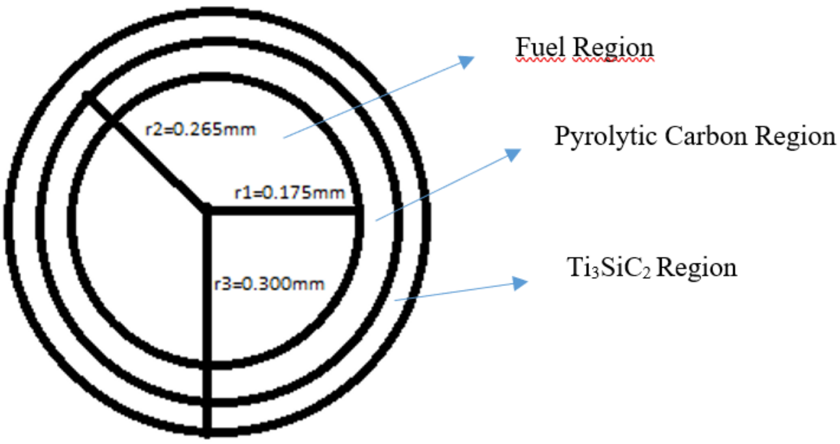


Fig. 5. TRISO particles of the fuel pellets model of fuel assembly

(Yakıt demetinde yakıt pelet modelinin TRISO parçacıkları)

In order to disperse the pebble on the pellet, Serpent disperse routine was used, so that no approximations used such as grow and shake algorithm. Three different qualities of graphite were used for the graphite blocks used in the reactor. These are 1.65 g/cm^3, 1.80 g/cm^3 and 2.16 g/cm^3 respectively. The effect of the quality of graphite used on the amount of burned thorium and the operating time of the reactor has been examined. In this study, the density of graphite used as a moderator has been taken as 2.16 g/cm^3, while making the main calculations, and SiC was preferred as the clad material. The neutronic calculations for heterogeneous 3D full core geometry, SERPENT Monte Carlo reactor physics burnup calculation code with ENDF/ B-VII cross section have been performed [16].

3. Results and Discussions (Sonuçlar ve Tartışma)

The neutronic calculations for a low power HTGR three dimensional heterogeneous full core were performed for various parameters, such as the density of the hexagonal graphite blocks and SiC and ZrC cladding materials in the fuel pellet. The Serpent continuous-energy Monte Carlo reactor physics burnup calculation code with ENDF/ B-VII data libraries have been used. During the course of calculations, the reactor power has been assumed as 60 MW$_{th}$.

In the study using the reactor core cell method [8], the initial infinite reactivity value was obtained then it was higher than the initial effective reactivity value of three dimensional heterogeneous full core method. Because reactor core cell method couldn't converge the neutron leakage exactly. When reactor core cell method has been used, it is observed that reactivity is more about 5 percent.

The effective reactivity has been determined as (k_{eff}-1)/k_{eff}) over operation period in the 3D heterogeneous full core method [17]. As shown in Fig.6, the results of the effective reactivity for different density of the hexagonal graphite blocks have been presented. The effective reactivity with increasing density of graphite has been increased. It is seen that when the quality of the graphite in the moderator increases, the neutron leakage decreases, therefore the initial reactivity value is higher. The long operating time of the reactor has been provided with increasing graphite density due to highest moderation. Also, SiC and ZrC cladding materials in fuel pellet are compared for the highest moderation situation as shown in Fig. 7. As illustrated in Fig 7., it is seen that Zr metal has a negative effect on reactivity. It has been observed that reactivity decreases by 2 to 3 percent when ZrC cladding is used in the reactor. This is because SiC has smaller neutron absorption cross sections than ZrC. There are also other advantages of using SiC compounds as clads. general chemical inertness, ability to withstand higher fuel burns and higher temperatures, exceptional inherent radiation resistance, etc [14].

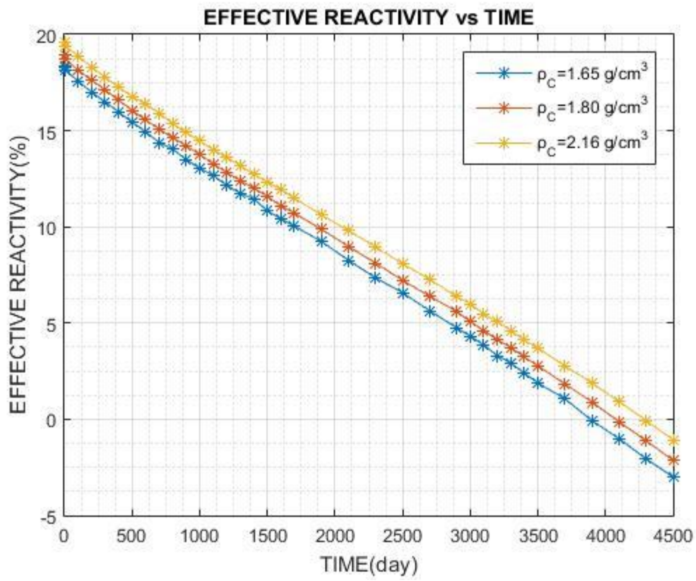


Fig. 6. Effective reactivity variations with different graphite density of HTGR full core

(HTGR tam çekirdeğin farklı grafit yoğunluğu ile etkin reaktivite değişimleri)

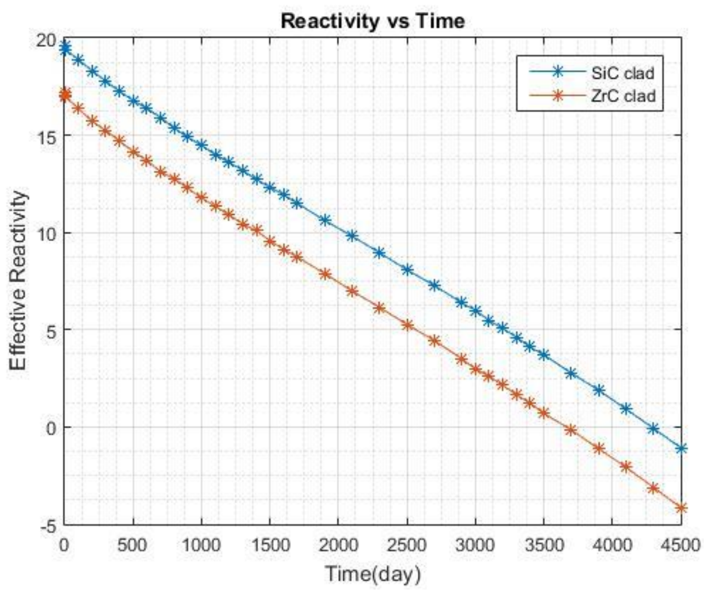


Fig. 7. Effective reactivity variations with different cladding material of HTGR full core

(HTGR tam çekirdeğin farklı kaplama malzemeleriyle etkin reaktivite değişimleri)

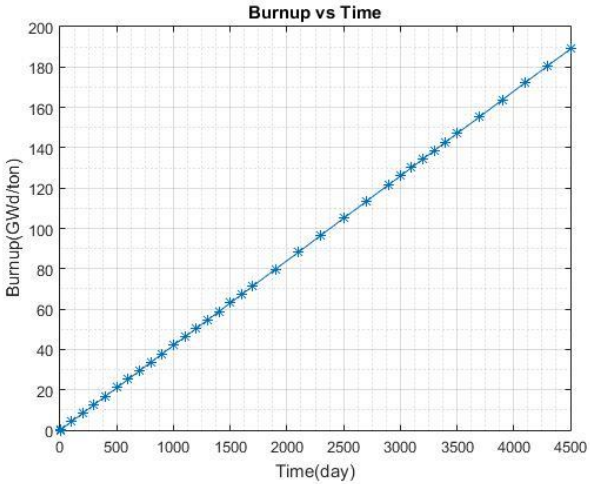
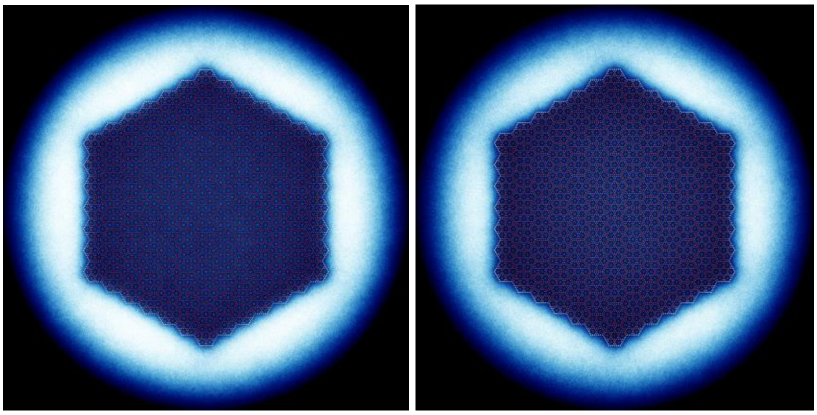


Fig. 8. Changes of the burnup values for 2.16 g/cm^3 graphite density of HTGR full core

(HTGR tam çekirdeğin 2,16 g/cm3 grafit yoğunluğu için yanma değerlerinin değişimi)



a) b)

Fig. 9. The images a) burning at the beginning, b) burning at the end of life of HTGR full core (Görüntü a) HTGR tam çekirdeğinde başlangıçta yanma b) işletim zamanı sonu yanma)

The SiC compounds have been chosen for all these advantages viz., increasing criticality and operation time in the neutronic analysis. As shown in Fig. 8., the burnup values over operation times have been performed. The burnup values have been obtained as 147 GWd/ton at 3500 days. The obtained results with reactor core cell method performed by I.V. Shamanin [8-9] have been compared with three-dimensional heterogeneous full core in this study. The obtained results have been verified with I.V. Shamanin [8-9]. Neutronic analysis of low power HTGR was made with a 3D heterogeneous model, and it was observed that the reactor worked up to 4500 days when the density of graphite used as a moderator in the reactor was 2.16 g/cm^3. Due to this, the burnup value when using higher quality graphite as a moderator is 189 GWd/ton end of life for using 3D heterogeneous full core calculations as shown in Fig. 8. Also, the burning images of the reactor on initial and final days are given as shown in Fig. 9.

As shown in Fig. 10., it was also observed that when using high quality graphite, the reactor thermalized and burned less thorium. According to the data given in Table 3, when the graphite density is equal to 2.16 gr/cm^3, 7.94 percent of the thorium in the fuel is burned. In addition, 6.9074x10^3 g ^{233}U is formed as a result of burning thorium as presented in Fig 10. Also, Plutonium isotopes changes have been given in Fig. 11. 239Pu isotope is decreasing with operation time, whereas the other isotopes of Pu are increasing. Approximately 3.78973x10^5 g Pu 239 is consumed in the reactor. In addition, there is a significant increase in the masses of Pu-240 and Pu-241 isotopes.

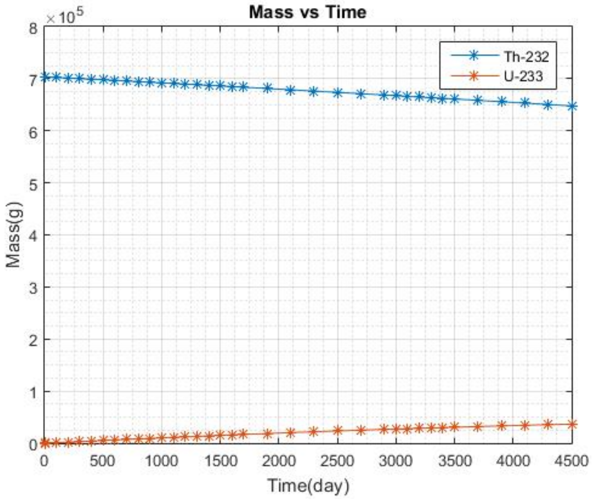


Fig. 10. Temporal variation of density (^{232}Th and ^{233}U) in the HTGR full core with SiC fuel pellet clad (SiC yakıt peleti kaplı HTGR tam çekirdeğinde geçici yoğunluk değişimi (^{232}Th ve ^{233}U))

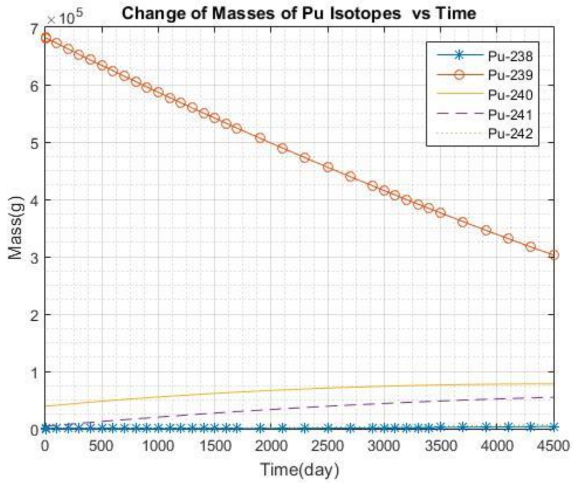


Fig. 11. Temporal variation of density (Pu isotopes) in the HTGR full core with SiC fuel pellet clad (SiC yakıt peleti kaplı HTGR tam çekirdeğindeki yoğunluğun (Pu izotopları) geçici değişimi)

Table 3. Percentages of Thorium Burned in Core with Different Graphite Density (Farklı grafit yoğunluğuna sahip çekirdekte yakılan toryum yüzdeleri)

Graphite Density(g/cm^3)	**Amount of Thorium Burned (%)**
1.65	8.5800
1.8	8.2974
2.16	7.9419

Finally, when investigation of the relationship between graphite density and thorium burning amount; the density of graphite is decreased whereas, the amount of incinerated thorium is increased. This is because the spectra of neutrons shift towards the fast region. Less control of neutrons increases the probability of fast fission.

4.CONCLUSIONS (SONUÇLAR)

In this study, neutronic analysis of low power HTGR was performed with a 3D heterogeneous full core model. The following conclusions can also be reached:

- The effective reactivity increases with the increasing density of graphite in the moderator.
- SiC, which has smaller neutron absorption cross sections has a positive effect on reactivity compared to ZrC.
- The burnup value has been computed as 189 GWd/ton and it was observed that the reactor operation time is up to 4500 days when the high-quality graphite used as a moderator.
- The 7.94 percent of the thorium in the fuel was burned when the high-quality

graphite and SiC clad of the fuel pellet were used. The thorium fuel utilization has been demonstrated successfully within the objective of generic investigations.

- Finally, drastic reduction of the nuclear waste material per unit energy output for final waste disposal through extended burn up.

DECLARATION OF ETHICAL STANDARDS
(ETİK STANDARTLARIN BEYANI)

we declares that the materials and methods they use in their work do not require ethical committee approval and/or legal-specific permission.

Bu makalenin yazarı çalışmalarında kullandıkları materyal ve yöntemlerin etik kurul izni ve/veya yasal-özel bir izin gerektirmediğini beyan ederler.

AUTHORS' CONTRIBUTIONS (YAZARLARIN KATKILARI)

***Ahmet ÇİFCİ*:** The author prepared the serpent code and ran it.

Adem ACIR: literature review and interpretation of results

CONFLICT OF INTEREST (ÇIKAR ÇATIŞMASI)

There is no conflict of interest in this study.

Bu çalışmada herhangi bir çıkar çatışması yoktur.

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