Study on MOX Core Characteristics of Experimental Power Reactor using MCNP6 Code

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Abstract. In experimental power reactor (reaktor daya eksperimental, RDE), a full MOX fueled core can be accommodated in its operation without significant modifications on the reactor core design, but the MOX core tends to produce less favorable safety features and deliver transient behavior into unwanted fatal accidents. This paper aimed to investigate the MOX core characteristics of RDE through a series of calculations with MCNP6 code and ENDF/B-VII library. The calculation results show that MOX core with $^{235}$U enrichment of above 5% can reach the criticality condition, maintain and run the reactor during the operation cycle. Utilizing MOX fuel in RDE with lower $^{235}$U enrichment will have a more negative impact on temperature coefficient of reactivity. The lower $\beta_{\text{eff}}$ makes the MOX core is more difficult to control, especially with low $^{235}$U enrichment. These results conclude that the selection of $^{235}$U enrichment in the MOX core must be carefully considered because it is one of the strategies to ensure the reactor safety criteria are fulfilled.

Keywords: MOX, core characteristics, experimental power reactor, MCNP6, ENDF/B-VII

1. Introduction

The sharply increase of world energy demand along with the rising of living standard of the world's population is a serious problem that must be solved. Meanwhile, the shrinking of fossil energy and the negative effects of fossil fuel consumption such as climate change, pollution, and others have become another very worrying problem in the recent decade. Nuclear energy which is free from air-pollution and green-house-gas is the most prospective energy option among various energy sources in overcoming the problem of increasing world energy demand in the future [1,2].

Pebble bed reactor (PBR), a type of the high-temperature gas-cooled reactor (HTGR), is one of the main candidates for the next Generation IV nuclear energy systems. The reactor uses graphite as neutron moderator and helium as coolant. The unique design of the PBR comes from the use of spherical fuel called pebble. This tennis-ball sized pebble contains thousands of TRISO coated fuel
particles distributed randomly in graphite matrix, and covered by graphite shell. TRISO particle comprises a small spherical kernel surrounded by several coatings designed to tolerate high burnup and prevent the release of fission products [3].

The main advantages of the PBR are the inherent safety features characterized by a strong negative temperature coefficient of reactivities, the large thermal inertia of the large graphite mass of the core and the fuel design retaining all fission products in the TRISO particles. These advantages insure no core damage and the core remains intact in any accident scenario that causes the reactor temperature increases up to 1600 °C. Another advantage of the reactor is the high coolant outlet temperature that produces high thermal efficiency in electricity production. The advantages of PBR are complemented by a fuel technology breakthrough that eliminates the need for shutdown of electricity and process heat for industrial applications such as hydrogen production, seawater desalination, enhanced oil recovery, and others.

Another advantage of PBR is its flexibility in term of type of fuel material, including thorium [4], plutonium [5], also rock-like oxide (ROX) [6]. Nowadays the mixed oxide (MOX) fuel is widely used in numerous light water reactors in various countries in Europe and Japan, but MOX fuel is still restricted to use in only one-third of their cores. The experimental power reactor (reaktor daya eksperimental, RDE) [7] is one pebble bed reactor type of high-temperature gas-cooled reactors which refers to the design and technology of HTR-10 China [8]. The HTR-10 was built based on German pebble bed technology by combining the AVR and HTR-Modul reactors. Like HTR-10, the construction and operation of RDE aims to acquire knowledge and experience in the design, construction and operation of high temperature reactors. Another goal is to demonstrate the modular HTR inherent safety features and to create facilities for producing experimental results.

In the RDE, a full MOX fueled core can be accommodated in its operation without significant modification on the reactor core design. The use of MOX fuel in the reactor core is very interesting because it is a way of utilizing surplus weapons-grade plutonium and an alternative to storage of surplus plutonium which would need to be secured against the risk of theft for use in nuclear weapons. However, the fuel load switched from UOX to MOX would change the operating characteristics of the reactor. The reactor control systems may need modification as plutonium isotopes absorb more neutrons than uranium fuels. The MOX core tends to produce less favorable safety features and deliver transient behavior into unwanted fatal accidents. Therefore, MOX core characteristics should be thoroughly examined [9,10].

This paper aimed to investigate the MOX core characteristics of RDE through a series of calculations with Monte Carlo transport code MCNP6 [11] and continuous energy nuclear data library ENDF/B-VII [12]. Some important reactor physics parameters were analyzed such as the effective multiplication factor \(k_{\text{eff}}\), the temperature coefficients of reactivity and the effective delayed neutron fraction \(\beta_{\text{eff}}\) for a variety of fuel enrichment.

2. RDE Reactor

The RDE reactor, which is planned to be built in Puspiptek area, Serpong, Tangerang Selatan, is designed for co-generation of electricity and district heating with 10 MW thermal power. The RDE has a cylindrical core with dimensions of 180 cm in diameter and 197 cm in average height. The core is surrounded by the top, bottom and side reflectors made of graphite as the main structural material in the reactor. The reactor shutdown system consists of 10 control rods and 7 small absorber balls located in the inner side of graphite reflector. The reactor is equipped by 3 channels for irradiation experiments located also in the inner side of the reflector. The helium coolant system consists of 20 helium flow channels located in the outer side of the graphite reflector. The helium enters to the reactor core at a temperature of 250 °C, flows downward through gap between pebbles and exits from the reactor at a temperature of 700 °C. The reactor design characteristics of RDE are given in table 1.

The fuel pebbles are loaded from the top and discharged from the bottom of reactor core. In RDE core management, each fuel pebble can be recirculated through the core five times in Multi-pass scheme until reaching their target burnup. The nominal volume of the core is 5 m³. The core including
a cone at the lower part of the core contains 27,000 fuel pebbles arranged randomly with a packing fraction of 0.61.

**Table 1.** The reactor design characteristics of RDE [7].

| Reactor parameter                      | Value          |
|----------------------------------------|----------------|
| Thermal power (MW)                     | 10             |
| Helium temperature at reactor inlet/outlet (°C/°C) | 250/700        |
| Helium pressure (MPa)                  | 3              |
| Helium mass flowrate at full power (kg/s) | 4.3            |
| Number of control rods in side reflector | 10             |
| Number of absorber balls in side reflector | 7              |

**Core specification**

| Core diameter/height (cm/cm) | 180/197 |
|-------------------------------|---------|
| Average power density (MW/m³)  | 2       |
| Number of fuel pebble in full core | 27,000 |
| Packing fraction of fuel pebble in the reactor core | 0.61 |
| Average discharge burnup (MWd/t) | 80,000 |
| Fuel loading scheme            | Multi-pass |

**Table 2.** Plutonium isotopic composition.

| Isotope | Pu composition (%) |
|---------|--------------------|
| ²³⁸Pu   | 2.68               |
| ²³⁹Pu   | 55.58              |
| ²⁴⁰Pu   | 23.08              |
| ²⁴¹Pu   | 11.98              |
| ²⁴²Pu   | 6.68               |

The fuel pebbles have two regions: fueled zone region of 5 cm diameter containing 8,335 TRISO particles and moderator region called graphite shell with thickness of 0.5 cm. Each TRISO particle is composed by a MOX fuel kernel in the center with ²³⁵U enrichment in uranium oxide of 5-20 % and plutonium fraction of 10 %, wrapped with four layers of the three isotropic materials: buffer layer made of carbon (C), inner layer of pyrocarbon (iPyC), ceramic layer of silicon carbide (SiC) and outer layer of pyrocarbon (oPyC). The layers of TRISO coated particle have the thicknesses of 0.009 cm, 0.0040 cm, 0.0035 cm, and 0.0040 cm. These coating layers act as an excellent barrier to retain the radioactive gaseous and metallic fission products and to prevent the release of fission products at temperatures up to and beyond 1600 °C. To ensure this temperature is never reached, the reactor is designed with a negative temperature coefficient of reactivity and passive heat transport mechanism for decay heat removal such as heat conduction, radiation, and nature convection [13]. The plutonium isotopic composition was adopted from Bende [14] as given in table 2. The detailed specifications of fuel pebble are summarized in table 3. Figure 1 illustrates the schematic view of fuel pebble in RDE.
Table 3. Fuel pebble specification.

| Fuel pebble                |                  |
|----------------------------|------------------|
| Pebble diameter (cm)       | 6                |
| Fueled-zone diameter (cm)  | 5                |
| Fuel mass per pebble (g)   | 5.68             |
| Graphite matrix/shell density (g/cm$^3$) | 1.73             |
| Natural boron impurity in graphite (ppm) | 1.30             |

| TRISO coated particle      |                  |
|----------------------------|------------------|
| Fuel kernel                |                  |
| Material                   | MOX              |
| Diameter (µm)              | 500              |
| Density (g/cm$^3$)         | 10.4             |
| $^{235}$U enrichment (%)   | 5-20             |
| Pu fraction in fuel (%)    | 10               |

| Coating layers             |                  |
|----------------------------|------------------|
| Buffer layer               |                  |
| Thickness (µm)             | 90               |
| Density (g/cm$^3$)         | 1.10             |
| iPyC layer                 |                  |
| Thickness (µm)             | 40               |
| Density (g/cm$^3$)         | 1.90             |
| SiC layer                  |                  |
| Thickness (µm)             | 35               |
| Density (g/cm$^3$)         | 3.18             |
| oPyC layer                 |                  |
| Thickness (µm)             | 40               |
| Density (g/cm$^3$)         | 1.90             |

Figure 1. Schematic view of fuel pebble [15].
3. Calculation Model

Unlike conventional reactors, such as pressurized water reactors (PWRs) and boiling water reactors (BWRs), modeling of the PBR is a challenge that requires special treatment because of its extra-complex geometry. The MCNP, which is well known as widely used and powerful Monte Carlo transport code, capable of treating this challenge because of its superior feature in modeling and performing calculation for complex heterogeneous geometries. The accuracy of the MCNP modeling in PBR simulations with double heterogeneity problem has been investigated through comparison of the results to other computational and experimental values in various studies [16-19].

![Image of MCNP6 modeling of TRISO particle in fuel pebble and fuel pebble in BCC lattice.](image)

(a). TRISO particle in SC lattice.  
(b). Fuel pebble in BCC lattice.

**Figure 2.** The MCNP6 modeling of TRISO particle in fuel pebble.

Initial step of RDE modeling begins with modeling a random distribution of TRISO coated particles in the fuel pebble as the first heterogeneity problem. The TRISO particle dispersed in graphite matrix was modeled with simple cubic (SC) lattice. This lattice was defined as a UNIVERSE. The fuel pebble was then modeled with repeated structure as provided in MCNP6 to distribute the 8,335 TRISO particles in the fueled zone. The repeated structure was constructed by UNIVERSE and combination of LATTICE and FILL options provided in MCNP6. The TRISO packing fraction in fuel pebble is 5.025 % which corresponds to SC lattice pitch of 0.19878 cm. The graphite shell covering the fueled zone with thickness of 0.5 cm was modeled to complete the fuel pebble model. In this model, the contribution of truncated particles on the spherical surface of the fueled zone, caused by the utilization of the repeated structure, is not considered because between uncorrected and with corrected simulation results are very close to each other and show insignificant difference. Moreover, the pebble boundary effect is only important for cell calculations and generally negligible for pebble bed core calculations [20].

The next step of RDE modeling is to model a random distribution of fuel pebbles in the reactor core as the second heterogeneity problem. The fuel pebbles arrangement in the reactor core was modeled with body-centered cubic (BCC) lattice comprising one pebble located in the center and one-eight pebble located in eight corners of the lattice. The helium coolant in the lattice was modeled outside these two pebbles. This lattice was defined also as a UNIVERSE. The BCC lattice pitch was chosen to be 7.18526 cm adjusted by pebble packing fraction in reactor core of 61 %. Figure 2 illustrates the MCNP6 modeling of TRISO particle in SC lattice and fuel pebbles in BCC lattice. The detailed explanation of this condition could be found in previous publications [21-30].

Like fuel pebble, the reactor core was then modeled by creating repeated structure to distribute 27,000 pebbles occupying a full core of 5 m³. The contribution of truncated pebbles on the cylindrical surface of the core caused by the utilization of the repeated structure, called the partial pebble, is eliminated by applying an exclusive zone of helium with a thickness of 3 cm around the core.
The exact representations of other reactor components such as graphite reflector side consisting of coolant channels, control rods and small absorber balls with their complex geometries are modeled in detail and explicitly, including the cone in the bottom of reactor core occupied by fuel pebbles also with the same packing fraction. Figure 3 illustrates the MCNP6 modeling of RDE. The isotopic concentration of TRISO particles with $^{235}$U enrichment of 5% are given in table 4. The isotopic concentrations of the graphite matrix and the graphite shell, which are identical, are given in table 5.

**Table 4.** Isotopic concentration of TRISO coated particle.

| Kernel MOX | $^{235}$U | $^{238}$U | $^{239}$Pu | $^{240}$Pu | $^{241}$Pu | $^{242}$Pu | $^{16}$O | $^{12}$C | iPyC/oPyC | SiC |
|------------|-----------|-----------|------------|-------------|-------------|-------------|---------|--------|----------|-----|
|            | $1.05701 \times 10^{-3}$ | $1.98295 \times 10^{-2}$ | $6.17287 \times 10^{-5}$ | $1.28018 \times 10^{-3}$ | $5.31604 \times 10^{-4}$ | $2.75936 \times 10^{-4}$ | $1.53861 \times 10^{-4}$ | $4.63797 \times 10^{-2}$ | $9.52614 \times 10^{-2}$ | $7.45040 \times 10^{-4}$ | $4.77590 \times 10^{-2}$ |
Table 5. Isotopic concentrations of the graphite matrix and the graphite shell [11].

|            | Graphite matrix | Graphite shell |
|------------|-----------------|----------------|
| $^{12}$C   | 8.67417×10$^{-2}$ | 8.67417×10$^{-2}$ |
| $^{10}$B  | 2.24401×10$^{-8}$ | 2.24401×10$^{-8}$ |
| $^{11}$B  | 9.03242×10$^{-8}$ | 9.03242×10$^{-8}$ |

4. Results and Discussions

The MCNP6 calculations were performed to estimate some important reactor physics parameters such as the effective multiplication factor ($k_{\text{eff}}$), the temperature coefficients of reactivity and the effective delayed neutron fraction ($\beta_{\text{eff}}$). The 10,000 neutron particles histories per cycle with 250 active cycles and skipped 50 cycles were simulated in the KCODE card before the active cycles begin. This card is used to monitor the neutron population changes and simultaneously stabilize the chain reaction in the reactor core. The initial fission source in the KSRC card was defined at the fuel kernel center and many individual source points to lead the calculation of reactor parameters from one cycle to the next cycle of fission reactions.

The continuous energy nuclear data library ENDF/B-VII was used in all calculations. The thermal scattering library $S(\alpha, \beta)$ was applied to consider the interaction of thermal neutrons with graphite moderator, graphite reflector, and graphite contained in the entire fuel pebble under the energy of ~4 eV. The calculation of effective delayed neutron fraction ($\beta_{\text{eff}}$) was conducted by applying the KOPTS card in the MCNP6 input data. The neutron transport simulations were performed by positioning all control rods completely withdrawn and placing 27,000 fuel pebbles in the reactor core. The outer boundary of the RDE reactor system was assumed as vacuum conditions.

The calculation result of the effective multiplication factor ($k_{\text{eff}}$) is shown in Table 6. This table confirms that MOX core with $^{235}$U enrichment of above 5% can reach the criticality condition, maintain and run the reactor during the operation cycle because its effective multiplication factor ($k_{\text{eff}}$) is greater than one. The MOX core with $^{235}$U enrichment of less than 5% can not be operated. It can be seen, the fuel pebble with higher $^{235}$U enrichment causes a higher value in $k_{\text{eff}}$ because of the higher thermal absorption cross section and the larger presence of the fissile isotope of $^{235}$U. The higher $^{235}$U enrichment hardens the neutron spectrum. In this calculation, the temperature was chosen to be 293 K.

Table 6. The effective multiplication factor ($k_{\text{eff}}$).

|            | $k_{\text{eff}}$       |
|------------|------------------------|
| UOX core   | 1.17856±0.00056        |
| MOX with $^{235}$U enrichment of 5% | 0.97750±0.00063     |
| MOX with $^{235}$U enrichment of 10% | 1.02111±0.00066      |
| MOX with $^{235}$U enrichment of 15% | 1.05144±0.00060     |
| MOX with $^{235}$U enrichment of 20% | 1.07874±0.00065      |

Temperature coefficient of reactivity plays an important role in the safety, control and operation of nuclear reactors. In PBR, moderator temperature coefficient (MTC) and fuel temperature coefficient, called Doppler temperature coefficient (DTC), are the most dominant two reactivity coefficients. Moderator temperature coefficient of RDE reactor was calculated by changing temperature from 293 K to 1200 K in moderator region and keeping temperature in other region constant (293 K). The MTC
values of UOX and MOX cores are shown in table 7. MOX cores show the stronger moderator temperature coefficients of reactivity (MTC) compared with UOX core. This is because of more sensitivity to neutron spectrum changes and dependences on thermal fission. MOX cores are more sensitive to moderator-temperature-induced transients compared with UOX cores.

Table 7. The moderator coefficient of reactivity (MTC, Δk/k K⁻¹).

| Core Type          | MTC  |
|--------------------|------|
| UOX core           | -2.86×10⁻⁵ |
| MOX with ⁰²³⁵U enrichment of 5 % | -4.68×10⁻⁵ |
| MOX with ⁰²³⁵U enrichment of 10 % | -4.26×10⁻⁵ |
| MOX with ⁰²³⁵U enrichment of 15 % | -3.67×10⁻⁵ |
| MOX with ⁰²³⁵U enrichment of 20 % | -3.60×10⁻⁵ |

Similarly, Doppler temperature coefficient of RDE reactor was calculated by varying temperature from 293 K to 1200 K in fuel region and maintaining temperature in other region constant (293 K). The Doppler temperature coefficients of reactivity, as shown in table 8, is strong in the MOX cores compared with UOX cores. The reason behind this fact is explained by higher number of resonance peaks resulted from more isotopes in the MOX fuel. These results suggest that utilizing MOX fuel in RDE with lower ⁰²³⁵U enrichment will have more negative impact on temperature coefficient of reactivity.

Table 8. The Doppler coefficient of reactivity (DTC, Δk/k K⁻¹).

| Core Type          | DTC  |
|--------------------|------|
| UOX core           | -3.31×10⁻⁵ |
| MOX with ⁰²³⁵U enrichment of 5 % | -5.94×10⁻⁵ |
| MOX with ⁰²³⁵U enrichment of 10 % | -5.24×10⁻⁵ |
| MOX with ⁰²³⁵U enrichment of 15 % | -5.16×10⁻⁵ |
| MOX with ⁰²³⁵U enrichment of 20 % | -4.82×10⁻⁵ |

The ability to control the reactor is determined by how much the effective delayed neutron fraction (β_eff) is. The β_eff is an important reactor parameter having to be investigated. The calculation results of β_eff for UOX and MOX cores are illustrated in table 9. The lower delayed neutron fraction of ⁰²³⁹Pu compared with ⁰²³⁵U is the reason why the MOX cores have lower effective delayed neutron fraction (β_eff) compared with UOX cores. MOX cores are therefore more difficult to control, especially with low ²³⁵U enrichment. The calculation of β_eff was performed at operation temperature of 900 K.

Table 9. The effective delayed neutron fraction (β_eff).

| Core Type          | β_eff          |
|--------------------|----------------|
| UOX core           | 0.00796±0.00070 |
| MOX with ⁰²³⁵U enrichment of 5 % | 0.00329±0.00040 |
| MOX with ⁰²³⁵U enrichment of 10 % | 0.00376±0.00048 |
| MOX with ⁰²³⁵U enrichment of 15 % | 0.00418±0.00057 |
| MOX with ⁰²³⁵U enrichment of 20 % | 0.00502±0.00059 |
5. Conclusion
Study on MOX core characteristics of RDE has been carried out through a series of calculations with MCNP6 code and ENDF/B-VII library. The calculation results show that MOX core with $^{235}$U enrichment of above 5% can reach the criticality condition, maintain and run the reactor during the operation cycle. Utilizing MOX fuel in RDE with lower $^{235}$U enrichment will have a more negative impact on temperature coefficient of reactivity. The lower $\beta_{\text{eff}}$ makes the MOX core is more difficult to control, especially with low $^{235}$U enrichment. These results conclude that the selection of $^{235}$U enrichment in the MOX core must be carefully considered because it is one of the strategies to ensure the reactor safety criteria are fulfilled.

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