Neutronic Calculation of Mixed Oxide Fuel for Gas-Cooled Fast Reactor using Monte Carlo code OpenMC

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Abstract. A fundamental aspect of nuclear power is using the prepared nuclear fuel once and then dumping it as waste, most of it can be recycled, thus closing the fuel cycle. The current means of doing this is by separating and recycling the plutonium. This plutonium is then blended with natural uranium to form mixed oxide (MOX) fuel. Neutronics calculations for the Gas-Cooled Fast Reactor are performed by OpenMC - Monte Carlo neutron and photon transport code. The parameter observed is the infinite multiplication factor (kinf), where it has been concluded that increasing the plutonium percentage has an impact on increasing the value. Depletion was carried out on the MOX composition with the best results, namely 9%, 10%, and 11% based on the value kinf ≈ 1. The depletion results also gave good results as shown by the cell successfully reaching a critical condition with an effective multiplication factor ≈ 1.

Keywords: neutronic, mixed oxide, OpenMC, infinite multiplication factor

1 Introduction

World energy needs continue to increase along with population growth and industrial development. Nuclear has been considered as an alternative because it has the potential to provide large and relatively clean energy. Nuclear power plants use nuclear reactions to produce heat which is then converted into electrical energy. Nuclear energy has several advantages that make it important in world and national energy supplies. Here are some important points of nuclear energy [1]:

1. Large Energy Capacity: Nuclear power plants can provide consistently large energy capacity, helping to meet growing energy needs at the national and global levels.
2. Low Greenhouse Gas Emissions: Nuclear energy produces low greenhouse gas emissions during its electricity generation process, helping to reduce the impact on climate change compared to fossil fuel power plants.
3. Diversifying Energy Supply: By having diverse energy sources, countries can reduce dependence on fossil fuels, increase energy security, and reduce vulnerability to fluctuations in energy prices and supplies.

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4. Energy Independence: Having a strong source of nuclear energy can help countries become more energy independent, reducing dependence on fossil fuel imports from other countries.

Despite these advantages, it is important to consider security aspects, radioactive waste management, and disaster risks associated with the use of nuclear energy for which computational simulation is a very appropriate first step [1-3].

Computational simulation is an important step in the long series of nuclear power plant developments. The need for systematic experiments with good composition to carry out technical procedures accurately is one of the reasons for the importance of carrying out this research [2,4].

The fuel pin is a small component of a large nuclear reactor system. A good reactor is built with a good core material composition, especially the fuel pin. Therefore, it is necessary to carry out research related to determining the appropriate fuel composition in this research, which will focus on mixed oxide (MOX) fuel by varying the percentage of plutonium [2-8]. The purpose of carrying out variations is to see what the value of the infinite multiplication factor is for each percentage of plutonium mixed [2,8]. In addition, variations will be made to the fuel volume fraction to obtain more varied results from different geometries [3,4].

OpenMC is the tool of choice for carrying out this research simulation. Apart from being an open-source nuclear computing platform, OpenMC is also a nuclear computing tool that applies the Monte Carlo method in its calculations [9,10]. In previous research, fuel pin calculations were carried out using SRAC, which applied the Collision Probability (CP) method. In contrast to the method in SRAC, the method applied in OpenMC is more realistic because the method truly describes the history of neutron travel from start to finish, which is why the computing process is longer than SRAC which uses the Collision Probability (CP) method in its calculations [6,13,14]. There have been several studies that have been carried out previously regarding neutronic analysis, geometric design, fuel comparison, and minor actinides using SRAC, OpenMC, MCNP, etc. at the core and fuel assembly level [2-8,11]. In this study, we will compare and select the fuel pin of a Gas Cooled Fast Reactor.

2 Theory and Methodology

2.1 Multiplication Factor (k) and Criticality

Multiplication factors in nuclear science can be divided into two based on the probability of neutron leakage, namely the effective multiplication factor and the infinite multiplication factor. The effective multiplication factor is a quantity that shows the ratio of number of neutrons that can be produced in one fission cycle versus the initial number of neutrons needed to trigger the fission reaction. Meanwhile, the infinite multiplication factor is the ratio between the number of neutrons produced at one time to the initial number of neutrons but ignoring the neutron leak factor ($P_{NL} = 1$)

Mathematically, effective multiplication factor can be written as

$$keff = k_{\infty}.P_f.P_t = \eta.\varepsilon.p.f.P_f.P_t \quad (1)$$

or

$$k = \frac{number\ of\ neutrons\ in\ \ one\ generation}{number\ of\ neutrons\ in\ the\ previous\ generation} \tag{2}$$

Based on the previous definition of infinite multiplication factor, equation 1 can be written as follows

$$kinf = k_{\infty} = \eta.\varepsilon.p.f \tag{3}$$

where η is the reproduction factors value, ε is the fast fission factor value, p is the resonance escape probability value, f is the thermal utilization factor value, P_f is the fast non-leakage probability value, and P_t is thermal non-leakage probability value [15].

Based on the multiplication factor value, there are three classifications, namely:

1. k > 1 (supercritical), meaning that the number of neutrons in one generation is greater than in the previous generation (uncontrolled neutron population).
2. k = 1 (critical), meaning the number of neutrons in one generation is the same as the previous generation.
3. k < 1 (subcritical), meaning that the number of neutrons in one generation is less than in the previous generation (the neutron population continues to decrease).

2.2 OpenMC - Depletion Calculation

Simulations use Monte Carlo code, the behavior of single particles cannot be predicted but can be determined by the average behavior of particles originating from the same source. If the probability distribution that shapes the particle's journey is known then the single process that is generated and collides with the atomic nucleus can be simulated directly with Monte Carlo. If there are enough particles to simulate this method, the average behavior can be obtained with small statistical errors guaranteed by the central limit theorem. To be more precise, the central limit theorem states that the sample average variance of several physical parameters estimated using Monte Carlo will be inversely proportional to the number of real numbers, for example, the number of particles that can be simulated in equation 4 [9,10].

$$\sigma^2 = \frac{1}{N} \tag{4}$$

where σ^2 is the sample mean-variance and N is a real number.

OpenMC, which is one of the tools that apply the Monte Carlo method, simulates one particle at a time, meaning that no more than one particle is tracked in one program example.

3 Design and Specification

The fuel pin design is the first step in designing a nuclear reactor. The fuel pin is composed of fuel material, cladding, and coolant. **Figure 1.** displays the visualization results of OpenMC plotting in a 2-D radial direction using Python Matplotlib. Another advantage gained from using OpenMC is in terms of visualization because it can immediately display the results of the design that has been created. After all, the language used by OpenMC in its programming is based on Python, where in Python there are various variations in plotting so that the resulting display can be more attractive.

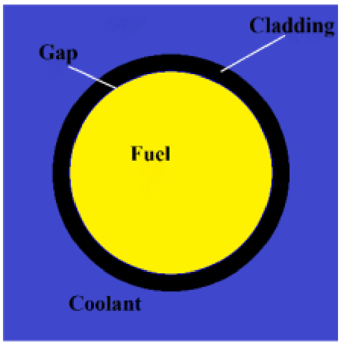

Fig 1. Fuel pin geometry design in the XY-axis with OpenMC

OpenMC classes Z-Cylinder and Z-Plane are classes used to describe fuel pin geometry. The Z-Cylinder class divides the area radially, while the Z-Plane divides it axially. The input given is the size of the external radius of each region. The fuel radius, gap, and cladding are respectively 0.416, 0.419456, and 0.483456, with a pitch of 0.9692 cm.

Table 1. Fuel Pin Information

Parameter	**Value**	**Unit**
Pin Radius	0.416	Cm
Inner Cladding Radius	0.419456	Cm
Outer Cladding Radius	0.483456	Cm
Side	0.74	Cm
Fuel Volume Fraction	65%	-

Table 2. Material Information

Parameter	Value	Unit
Pin Fuel	(U, Pu)O2	-
Cladding	SS 316	-
Coolant	Helium	-
Variations in Plutonium Fractions	0% (UO2) to 14%	wo

Table 1 contains information on the physical parameters of the fuel pin. The volume fractions of fuel, gap, cladding, and coolant are 65 percent, 0.54 percent, 10 percent, and 24.46 percent, respectively. We did not make changes or variations to the geometric size or volume fraction of the fuel pin so that the visualization of the plotting image remains the same as in **Figure 1.** Table 2 contains information about the materials used [4,6,16]. The material compositions used in the Fuel Pin, Cladding, and Coolant are Mixed Oxide (MOX), Stainless Steel SS 316, and Helium, respectively.

Apart from that, the fuel cell depletion process will be carried out on the fuel cell composition with good kinf results according to the criticality classification. In carrying out the depletion process, it is necessary to determine and initialize the power and time step in our OpenMC program. So we set a power of 250 Wth, which is 1/6 of the power normally used to deplete a small modular reactor core. Meanwhile, we set the time step for 180 days or six months.

4 Results and Discussion

OpenMC is capable of producing very diverse outputs such as effective multiplication factor, flux, fission reaction rate, neutron production rate, and other parameters. However, in this study, we only present information on the infinite multiplication factor as a parameter for describing the MOX fuel profile. We obtained these output parameters from the results of running the program with particle, batch, and inactive settings of 1000, 100, and 10, respectively. In this study, ENDF/B VIII.0 was chosen as the cross-section data for running the program, where ENDF/B VIII.0 is the most recent ENDF data.

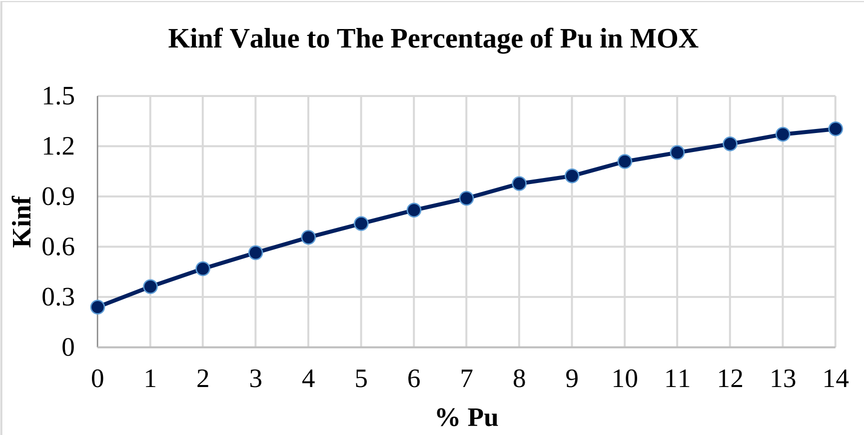

Fig 2. kinf value to the percentage of Pu in MOX

Figure 2. displays a comparison of the kinf value to the percentage of Pu in MOX. It can be seen that there is an increase in the kinf value as the percentage of Pu used increases. Theoretically, increasing the percentage of the Pu fraction in MOX will have an impact on increasing the fissile content. The research results successfully showed that critical conditions occurred starting when the Pu percentage was 9% at a fuel volume fraction of 65%.

MOX conditions with Pu 0% can be defined as the fuel used being Natural Uranium. Natural Uranium only contains 0.7% U235, which is the only fissile isotope in Natural Uranium. Because of this small amount of fissile content, the fuel pin design without Pu content is far from the critical condition with a kinf value of 0.24041, or what is usually called a subcritical condition. Furthermore, the Pu percentage of 1% to 8% is still below 1. For the percentage of 8%, it is almost close to critical conditions; apart from the fissile content factor, the pin size also influences the kinf value. The kinf value at a Pu percentage of 8% is 0.97772. If the size of the fuel rod is increased, the kinf value will certainly increase, and it is possible that MOX with Pu 8% will be in a critical condition. A good kinf result is a Pu composition of 9% to 11%. Meanwhile, for a composition of 12% to 14%, the kinf value is > 1, or supercritical. If at the cell level, the neutron ratio of neutron production is already high, of course this will also have the same impact at the core level. The highest kinf value was obtained at 14% Pu composition, namely 1.30297. Several other studies that have been carried out previously also provided significant results when increasing the fissile Pu content in MOX fuel which had an impact on increasing the multiplication factor value [5,11,12].

From the results of this research, we believe that Pu with a percentage of 9%,10%, and 11% is the best result for use at the core level with power (P ≤ 250 MWth) because MOX with a Pu percentage below 9% will have subcritical conditions in the first few year operation. Meanwhile, if Pu is above 11%, the core will be in a supercritical condition for a long time, even though neutron production can be controlled. In this research, we do not discuss the technical aspects of controlling neutrons because we only discuss fuel cell design.

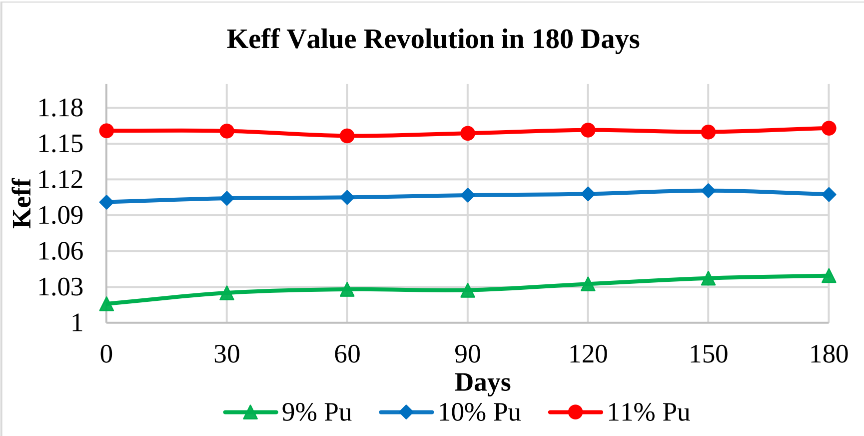

Fig 3. keff value revolution on MOX pin cell with Pu composition percentages of 9%, 10%, and 11% for 180 days using OpenMC

Figure 3. is an explanation of the depletion results of a previously designed pin cell which is a fuel with a good composition based on the kinf results that have been obtained. Depletion is carried out to find out whether the fuel if burnup is carried out, is capable of being in a critical condition from the start of operation. Based on the results obtained, it is known that the three compositions of the Pu composition variation can reach critical conditions from the start of the operation. Following the Pu content in each pin cell, the highest keff was obtained by Pu 11%, then below that was Pu 10%, and finally Pu 9%.

During six months of burnup, the highest keff point was obtained by Pu compositions of 9% and 11% in the same month, namely the sixth with respective values of 1.03945 and 1.16314. Meanwhile, the 10% Pu composition reached its highest point in the fifth month, namely 1.11072.

4 Conclusion

Initial investigations of the MOX pin cell design using OpenMC have been carried out by experimenting with variations in the Pu composition in MOX from 0% to 14%. Pin cell design with kinf in critical conditions (kinf ≈ 1), namely 9%, 10%, and 11%, with respective values of 1.02185, 1.10806, and 1.16153. We have also succeeded in carrying out depletion or burnup for 180 days on three pin cell designs with Pu 9%, 10%, and 11% . All three designs can reach critical conditions from begin of life (BOL) conditions up to 180 burnup days.

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