Comparison of Boron Carbide, Gadolinium Oxide, and Hafnium as Qualified Molten Salt Reactor’s Control Rods Material

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Abstract. The development and research of the Molten Salt Reactor (MSR) has recently seized the attention. Lots of MSR designs have been modeled based on its materials, neutronic behaviour, thermal-hydraulic behaviour, and particularly its safety systems. A reactor’s core has been modeled based on the design of ThorCon Reactor using Monte Carlo N-Particle 6 computational code with BeF₂-NaF-UF₄-ThF₄ mixture as the fuelsalt. The core contains 84 hexagonal fuel logs and a hexagonal control rod log. This research compared three different materials of control rods, i.e. B₄C, Gd₂O₃ and Hf. The comparison between those materials are seen according to reactor’s criticality. The \( k_{\text{eff}} \) at fully withdrawn position is 1.01887 that indicates a critical condition. When the control rods are fully entered the \( k_{\text{eff}} \) are (0.98293 ± 0.00012); (0.97386 ± 0.00011); (0.99203 ± 0.00012) for control rods’ materials in sequence B₄C, Gd2O3 and Hf. The decrection of the criticality shows the materials’ ability to absorb the neutron. The lower the criticality, the better material’s absorption ability.

1. Introduction
Molten Salt Reactor (MSR) is a nuclear fission reactor that uses mixture of liquid salt as it fuel and primary coolant. MSR is classified by the International Atomic Energy Agency (IAEA) as one of the fourth generation reactors because it prosperity to fulfills objectives that related to the safety, reliability, sustainability, and minimization of radioactive waste [1]. The ThorCon reactor is a trade name of MSR by US company named Martingale Inc. The ThorCon reactor has four modules in a suite that will produce 1000MWe (4 × 250 MWe) power [2].

Reactor criticality is a condition that must be known and monitored from a nuclear reactor. This value shows the comparison between number of neutrons at one generation and previous generation conditions. Critical condition marked by the \( k_{\text{eff}} = 1 \). If \( k_{\text{eff}} > 1 \), referred to as supercritical condition, otherwise when \( k_{\text{eff}} < 1 \) referred to as subcritical condition. The reactor that has just started up is in supercritical condition, slightly maintained above critical during operation and heading subcritical if it will shutdown. One of the quantities that can be derived from the \( k_{\text{eff}} \) is reactivity. Reactivity is the fractional change in neutron population per generation [3].
MSR has three shutdown systems [4]. The first system is the adjustment of the MSR fuel composition during the reactor operation, so that over time the reactor will shutdown by itself. The second is drainage system of MSR that will empty out the fuel inside the core and temporarily store it in the drain tank. The third system is a high speed shutdown system or usually called scram using the control rods.

Although MSR can shutdown by itself [4], the control rods still has important role to anticipate the disturbance that causes the reactor needs to be shutdown quickly so that no nuclear accident occurs. So, research of the right material to be used as MSR control rods is very interesting to do.

The control rod has three main functions, that is as reactivity compensation during reactor operation, to control the start and stop for normal operation, and for rapid shutdown in case of abnormal conditions. The main requirement for a good control rod is to have a large neutron absorption cross section. Especially for MSR, control rods must be resistant to corrosion, have a high thermal conductivity values to prevent excessive expansion and high boiling points so that control rods can be used at high temperatures [5], because MSR operates at high temperatures of 704° C or 977K.

Some materials that can be used as control rods are silver, indium, boron, cadmium, gadolinium, and hafnium [3]. Some interesting materials to study are boron carbide (B₄C) that used in Kartini reactor, gadolinium oxide (Gd₂O₃) that commonly used in CANDU type reactors, and hafnium (Hf) which are usually used as control rod materials in BWR and PWR type [6] [7]. The characteristics of the three materials are presented in the Table 1. From the table, it can be seen that Gd₂O₃ has larger absorption cross-sectional value than B₄C, but the thermal conductivity is smaller. Whereas Hf has a boiling point that much higher than both Gd₂O₃ and B₄C, so Hf can also be a good candidate to be the MSR control rods material.

| Parameters                      | Material      |
|---------------------------------|---------------|
| Absorption cross section (barns)| B₄C 49153     | Gd₂O₃ 500 |
| Thermal conductivity (W/mK)    | 29            | 10.6 23  |
| Boiling point (K)              | 3773          | 3273 4876 |
| Solubility                     | No            | No No  |

Table 1. B₄C, Gd₂O₃, dan Hf characteristics [7] [8]

Seen from the characteristics of these materials, it is necessary to compare the performance of B₄C, Gd₂O₃, and Hf as the most appropriate control rods for MSR in terms of their effect on the criticality value of the reactor. In this simulation, reactor criticality is calculated when at the fully up and spontaneously fully down position, without the releasing process of control rods.

To ensure the safety of the reactor, in a previous study [9], shutdown margin (SDM) and shutdown margin one stuck rod (SDM OSR) was also calculated to determine the distance from the reactor’s critical condition to the subcritical conditions where the control rod was inserted into the reactor. The change of negative reactivity is inversely to the value of SDM, when the negative reactivity gets smaller, the SDM gets bigger. The minimum value of SDM for power reactors is 750 pcm or 0.75%Δk/k [10].

This simulation uses Monte Carlo N-Particle-6 (MCNP6) computational code that adjust the Monte Carlo method. The Monte Carlo continuous energy method is one of the reliable methods for transporting particles such as neutrons, photons, and electrons in complex three-dimensional systems. This method is used because it can traces particle form it birth to death [11].
2. Methods
Figure 1. showed the flowchart procedure of this research.

Figure 1. Flowchart of the research procedure

MSR-ThorCon core geometry is modeled in Visual Editor (VisEd) Program based on the data in the MSR-ThorCon Design Control Document [2]. The MSR-ThorCon core consists of Pot made of stainless steel SUS316H, shields made of B$_4$C, graphite reflectors and moderators, 84 fuel logs with the following composition: BeF$_2$-NaF-UF$_4$-ThF with U-235 that enriched to 19.75%, and one control rods log in the middle of the core as in Figure 2. A control rods log contain a fixed graphite regular rod in the middle that always in fully down position, and surrounded by three shutdown rods with material to be varied with B$_4$C, Gd2O3, and Hf. After the core is done, $k_{eff}$ calculation command added through Notepad++ program, then run the MCNP6.

Figure 2. MCNP6 geometrical model of MSR-ThorCon [2]
After the geometrical model made, the $k_{\text{eff}}$ calculation command added through Notepad++ then the control rod’s material and temperature are varied and added to the script. After all the script are processed to get the results that is $k_{\text{eff}}$ value then analyzed. The $k_{\text{eff}}$ value also used to calculate the SDM and SDM OSR with this equation:

$$\text{SDM} = \rho_{\text{total rod}} - \rho_{\text{excess}}$$  \hspace{1cm} (1)

$$\text{SDM OSR} = \rho_{\text{total rod}} - \rho_{\text{excess}} - \rho_{\text{max}}$$  \hspace{1cm} (2)

Results and Discussion

The criticality calculation was conducted by KCODE calculation where $2.10^6$ particles are simulated with 250 cycles and 35 of the being skipped, with an estimated $k_{\text{eff}}$ value of 1.0. This calculation takes 887 minutes of simulation time with an Intel Core i3 PC processor. ThorCon operating temperature is 977K, but the MCNP data is not available for these temperatures so that the temperatures used 900K and 1200K. The $k_{\text{eff}}$ value at 977K is calculated using the interpolation equation. The $k_{\text{eff}}$ value when all shutdown rods are in the fully withdrawn position and when the shutdown rods dropped one by one to the core for each temperatures and each materials are shown in Table 2.

| Temperature (K) / $k_{\text{eff}}$ | Regular rod | Shutdown rod |
|------------------------------------|-------------|--------------|
|                                    | BaC         | Gd2O3        | Hf           |
| Amount                             |             |              |              |
| 900                                | 1.02179     | 1.01139      | 0.98802      | 1.00817 | 1.00399 | 0.98058 | 1.01281 | 1.00996 | 0.98850 |
| 977                                | 1.01885     | 1.00886      | 1.00263      | 0.98293 | 1.00608 | 0.99917 | 0.97386 | 1.00110 | 1.00757 | 0.99203 |
| 1200                               | 1.01035     | 1.00154      | 0.99124      | 0.96822 | 1.00005 | 0.98522 | 0.95443 | 1.00590 | 1.00065 | 0.97330 |

Table 2. $k_{\text{eff}}$ value for each variation

Figure 3. shows the comparison of $k_{\text{eff}}$ value with varied materials at 977 K. This study focus on temperature of 977K because it is the MSR-ThorCon operating temperature.
From the Figure 3-5, it can be seen that the addition of control rods to the reactor core can cause a decreation in $k_{eff}$ value of the MSR-ThorCon, because the control rods is absorbing neutron. The initial $k_{eff}$ of the reactor when no control rod is inserted is 1.01885, which indicates the reactor is in critical condition.

When all control rods are inserted, the criticality value of the reactor decreases to subcritical. The $k_{eff}$ with B$_4$C rods decreased to 0.98293 and the excess reactivity value of 1.7 %$\Delta k/k$. The $k_{eff}$ with Gd2O3 rods becomes 0.97286 with the excess reactivity of 2.7 %$\Delta k/k$. The Hf rods decreased the $k_{eff}$ value to 0.99203 and excess reactivity of 0.80 %$\Delta k/k$. From these results it can be seen that the material which has the biggest excess reactivity is Gd2O3 [7] [8]. So it can be said that the best control rods material for MSR-ThorCon is Gd2O3 because the control rods is only used to shutdown the reactor under certain conditions that can be dangerous [2] so the control rods must be able to absorb large amount of neutrons quickly.

To find out whether the these material can guarantee the safety of the reactor in case of emergency and all the control rods must be inserted to the core, the shutdown margin (SDM) is calculated. Other than that to anticipate if one of the control rods fails to enter the core, the shutdown margin one stuck rod (SDM OSR) is also calculated and the results are shown in Table 3.

| Calculation | %$\Delta k/k$ | B$_4$C | Gd2O3 | Hf |
|-------------|---------------|--------|--------|----|
| SDM         | 1.7           | 2.7    | 0.8    |    |
| SDM OSR     | 0.73          | 1.4    | 0.04   |    |

The results of SDM calculation of the B$_4$C, Gd2O3, and Hf rods shows that their values are above the minimum limit that has been set for power reactors. For the SDM OSR values, only Gd2O3 rods that qualified because its above the limit. B$_4$C and Hf rods are not qualified enough because theirf SDM-OSR values are below the limit. So it can be concluded that the most qualified materials for MSR-ThorCon’s control rods is Gd2O3 because it is safe for shutdown in case of an emergency.

**Conclusion**

Amongst the three control rod materials compared in this study, the best material used for MSR-ThorCon is Gd2O3, because the Gd2O3 rods has the best reduction $k_{eff}$ reduction of 0.97386, compared to $k_{eff}$ with B$_4$C rods that is 0.98293 and Hf which is 0.99203. In terms of the shutdown margin and shudown margin one stuck rod values, it can be said that the reactor is safe to go to shutdown because the value is above the minimum limit that has been set.

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