A Comparative Study of Th-U$^{233}$ and Th-Pu Molten-Salt Reactor (MSR) with 2-region core

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Abstract. Sustainable closed fuel cycle and inherent safety are one of the key aspects of Generation IV reactor design. Hence Molten salt reactor (MSR) is chosen as one of the candidates of Generation IV reactor concepts. FUJI-U2 or MSR-2R is a 2-region core MSR design that was proposed as a possible simplification of FUJI-U3 (3-region core). Taking into consideration that uranium$^{233}$ doesn’t exist naturally, FUJI-U2 utilize both plutonium and uranium$^{233}$ as a fissile material. To understand the characteristics further, a comparative study of 2-region core MSR with Th-U$^{233}$ and Th-Pu as fuel has been carried out. Nuclear analysis code SRAC2006 with the nuclear data library of JENDL4.0 was used, and CITATION was employed to validate the core. The design parameters set for each region are fuel composition, core radius, and fuel fraction. The simulation burn-up calculation is set to 2000 days in total, with 21 step each for 100 days cycle. Neutron multiplication factor, fuel elemental, burn up calculation, conversion ratio, and neutron flux in each core will be discussed.

1. Introduction
Sustainability, economics, safety, and proliferation resistance are the four pillars of Generation IV development[1]. One of the chosen candidates for advanced reactor concepts at the Generation IV (GENIV) International Forum is the Molten Salt Reactor (MSR). MSRs are liquid-fueled reactors that have various applications such as actinides burner, electricity and hydrogen producer, and can be use as a breeder reactor.

Small MSRs of 150e200 MWe (FUJI-II, FUJI-12 and FUJI-U3) have been proposed in Japan. FUJI-12 is a simple 1-region core, and it attained a high conversion ratio of 0.92 by the batch chemical processing in every 7.5 years. However, it appears that every 15 years FUJI-12 has to replace the graphite moderator and this may cause additional maintenance work and cost. K. Mitachi et al.[2] proposed a small MSR (FUJI-U3) with a 3-region core design concept in order to eliminate graphite replacement by reducing the maximum neutron flux and flattens it. The study result showed that graphite replacement is not necessary until 30 years of operation. Then Y. Honma et al., investigated the possibility of a two region core design concept for the simplicity. Using one energy group neutron
diffusion theory and assuming bare reactor. The optimization of the actual core configuration was searched by a nuclear analysis code SRAC2002 with the nuclear data library of JENDL3.3 [3]. In this paper we conducted a study of the nuclear data from the proposed design and compare the result of each fuel (Th-U\textsuperscript{233} and Th-Pu).

2. Design Specifications of FUJI-U2/MSR-2R

In the fuel cell calculation, the temperature of the fuel cell (fuel salt and graphite moderator) is assumed to be 900 K, which is a mean value between core inlet and outlet. As for the core R - Z calculation, the entire core temperature is also assumed to be 900 K. Design parameter and fuel cell models can be seen in Table 1 and 2 respectively.

| Reactor vessel | Core1 | Core2 |
|----------------|-------|-------|
| Diameter (m)   | 3.58  |       |
| Max. Radius/height, (m) | 2.40/2.20 | 3.00/2.20 |
| Fuel duct Width (m) | 0.04 |       |
| Reflector Thickness (m) | 0.5 |       |
| Geometrical Buckling | 7.49950 $\times 10^{-4}$ |       |

| Table 2. Design parameters of fuel cell models (MSR-2R)[3]. |
|----------------|-----------|-------------|----------------|
| K\textsubscript{inf} | d(bore)/2 (cm) | Fuel (vol%) | K\textsubscript{eff} (all core) |
| MSR-2R-U3 | | | |
| Core1 | 1.02730 | 5.10 | 31.5 | 1.003088 |
| Core2 | 1.11701 | 3.95 | 18.9 | |
| MSR-2R-PU | | | |
| Core1 | 1.01957 | 4.75 | 27.3 | 1.003006 |
| Core2 | 1.08729 | 4.40 | 23.4 | |

Figure 1 below display the reactor configuration in meshes. Notice that the core is radially divided into two regions, aimed to flatten the neutron flux which will directly affect the graphite life. Core1 and core 2 radiuses and fuel volume fraction used in the study for each fuel is shown in table 2 above. Figure 1 also shows the flow path between core 2 and the graphite reflector, as well as the fuel duct at the bottom and top of the core. The collision probability routine PIJ is used with 107 energy groups for unit fuel cell model with nuclear library of JENDL3.3 that can be seen in figure 2.
3. Nuclear Data Studies

To understand the characteristics of uranium and plutonium fueled 2-region core MSR, a comparative study of has been carried out. With the fuel cycle set to 21 each for 100 days. The objective of the nuclear data studies in this case is to find the neutron multiplication factor, fuel elemental, burn up calculation, conversion ratio, and neutron flux in each core for both MSR-2R-U3 and MSR-2R-PU. Nuclear analysis code SRAC2006[4] with the nuclear data library of JENDL4.0[5] was used, and CITATION was employed to validate the core. Fuel composition used in this study is referencing to the previous study done by Y.Honma et al.,[3] for Th-Pu as shown in table 3. As for the composition for Th-U$^{233}$, because it is not stated in the study done by Y.Honma et al., in this study the composition is the same as previous study done by K.Mitachi et al.,[2] as shown in table 4. Design parameters used in this study can be seen in table 5 below.

| Compositions | Fuel salt (mol%) |
|--------------|-----------------|
| LiF          | 71,76           |
| BeF$_2$      | 16,0            |
| ThF$_4$      | 9,0             |
| $^{238}$UF$_4$ | 1,51           |
| $^{238}$PuF$_4$ | 0,034         |
| $^{239}$PuF$_4$ | 1,09          |
| $^{240}$PuF$_4$ | 0,33           |
| $^{241}$PuF$_4$ | 0,20           |
| $^{242}$PuF$_4$ | 0,068          |

Table 3. MSR-2R-PU fuel compositions[3]

| Compositions | Fuel salt (mol%) |
|--------------|-----------------|
| LiF          | 71,78           |
| BeF$_2$      | 16,0            |
| ThF$_4$      | 12,0            |
| $^{233}$UF$_4$ | 0,22           |

Table 4. Fuel compositions of Th-U$^{233}$ MSR[2].
4. Results and Discussions

4.1. Multiplication Factor
The first crucial result discussed in this paper will be the multiplication factor. Neutron population is a key point to maintain the fission chain reaction, so quantitatively a multiplication factor is used as a tool to analyze the fission chain reaction. In an infinite reactor, the neutron loss consists of only neutron absorption and expressed as $K_{inf}$. But this is not the case for actual reactors (which has limited size) so taking into account the ratio between neutron production and loss or $K_{eff}$, is the effective neutron multiplication factor. If $K_{eff} = 1$, the number of neutrons is constant in the reactor, implicates that the fission rate is constant, and the constant energy release continues. This condition is ideal to achieve a thermal reactor in a critical state. If $K_{eff} < 1$, reactor is in subcritical state, which indicates the declining population of neutrons (gradually) with progression of the fission chain reaction. If $K_{eff} > 1$, the chain reaction increases, and the reactor is supercritical [6]. Figure 3 and Figure 4 show the result of $K_{inf}$ value of each core and $K_{eff}$ respectively. Figure 3 display the highest $K_{inf}$ that was achieved by core 2 using U\textsuperscript{233} fuel and notice that at the EOL (End of Life), the core is capable to maintain the critical state of the reactor ($K_{inf} ≥ 1$). Core 1 with U\textsuperscript{233} fuel is also showing a steady critical state in the case of $K_{inf}$. $K_{inf}$ of core2 plutonium fuel from day 1500 to EOL is in subcritical state ($K_{inf} < 1$), whilst in core1 plutonium in the first 500 operational day had already decreasing to subcritical state.

![Figure 3. K-inf of each core and fuel.](image1)

![Figure 4. K-eff for each fuel.](image2)

Because in the $K_{inf}$ calculation neutron loss or leakage is not taken into account, collectively core1 and core2 plutonium fuel had a relatively low $K_{inf}$ (compare to core1 and core2 U\textsuperscript{233} fuel) resulting in the rapid decline of $K_{eff}$ as shown in figure 4. The condition where $K_{eff} = 1$ is satisfied at the BOL (Beginning of Life) until 500 days operation and continue to decline, reaching 0.96 at the EOL. It is
clear from figures 3 and 4 below that to use the proposed plutonium fuel compositions; some adjustment is needed so that the fissile content can satisfy the critical state for the reactor to operate according to the desired operation time. Table 6 below provide the multiplication factor discrepancies from the reference study done by Y. Honma et al.[3]. The $K_{\text{inf}}$ acquired from the simulation is in $10^{-2}$ order smaller than the reference, this contributes directly to the noticeable difference of the $K_{\text{eff}}$ value for each fuel scenario. Different usage of JENDL is probably the cause of the overestimation of $K_{\text{inf}}$ and $K_{\text{eff}}$ values.

Table 6. Multiplication factor difference.

| Study Result          | Core1  | Core2  |
|-----------------------|--------|--------|
| Y. Honma et al.[3]     | 1,02730| 1,0320 |
| MSR-2R-U3 $K_{\text{inf}}$ | 1,11701| 1,1222 |
| MSR-2R-PU $K_{\text{inf}}$ | 1,01957| 1,01864|
| MSR-2R-U3 $K_{\text{eff}}$ | 1,003088| 1,026141|
| MSR-2R-PU $K_{\text{eff}}$ | 1,003006| 1,02751|

4.2. Elemental Composition

Fuel behavior can be predicted by the heavy nuclide composition. The compositions then will affect the reactor performance and the nuclear waste compositions [7]. Elements in the periodic table from actinium and upwards are classed as actinides. Major actinides are Uranium (U) and Plutonium (Pu) are two of principal element in nuclear fuel that classed as major actinides. While neptunium (Np), americium (Am), and curium (Cm) are normally taken as minor actinides (MA)[8]. Figure 5 and 6 below shows the elemental composition of core1 and core2 of each fuel, respectively. From the figure it is clear that each core consists of Thorium $^{232}$, Protactinium (PA), U, Np, Pu, Am, and Cm. This is the result of nuclear transmutation mechanism, where an element is transmute into other lighter element, induced by nuclear chain reaction such as neutron capture, or $\alpha$ and $\beta$ decays. Clearly thorium as the main fuel component has the highest composition, as shown in figure 5 and 6 below.

Figure 5. Core1 uranium fuel (a) and plutonium fuel (b) elemental compositions.
Figure 6. Core2 uranium fuel (a) and plutonium fuel (b) elemental compositions.

From the perspective of MA composition, figure 5(a) has a higher production of neptunium compared to (b), while figure 5(b) is dominated by americium. Because of its long half-life, neptunium is considered to be a significant contributor to long-term radiotoxicity. Although americium isotopes may have a shorter half-life than neptunium, it is considered as a prime candidate for transmutation, because of its significant contribution to gamma activity and radioactivity [8]. In Figure 6, it displays elemental compositions for core2 of each fuel. It is observed that both neptunium (figure 6(a)) and americium (figure 6(b)) are the same main MA product. This information can determine the possibility and the potential to be use as recycled fuel.

4.3. Conversion Ratio and Burn-up
Nuclear stability is guaranteed when the reactor is capable to convert the fertile materials into the fissile materials [7]. The conversion process is called conversion ratio (or sometimes breeding ratio), B.R or C.R, is defined as the average number of fissile atoms produced in a reactor per fissile fuel atom consumed. If C.R = 1, this will read as an infinite amount of fertile material can be converted in a given amount of fuel [9]. The C.R value of each core for each fuel scheme is presented in figure 7 below.

Figure 7. Uranium fuel (a) and plutonium fuel (b) Conversion ratio of each core.

Figure 7 display the distinctive behavior of C.R in each fuel case. In figure (a) Uranium fuel have a higher C.R value than plutonium fuel as high as 1,10 for core1 for the first 500 days, meaning that uranium fuel for the case of core1, have a good conversion abilities. Although the C.R for core1 is declining as it reached the EOL, the C.R value is still bigger than 1. On the contrary, core2 started at 0.9 for the first hundred days of operation and keep increasing until it reaches the core EOL but the...
C.R > 1. On the contrary, the increase in C.R is linear for both core1 and core2 in figure (b). Core1 have a higher C.R value than core2, starting at 0.81 at the BOL (C.R core2 is 0.74). Both core that uses plutonium as a fuel are incapable to sustain the reactor stability during operation, the consumed fissile atoms are higher than the fissile production.

Figure 8 show the burn-up results for each case. Fuel burn-up and core reactivity is closely linked to each other. Burn-up determine the amount of available fuel, affecting the reactor reactivity. Burn-up analysis is crucial to better understand how the kinematic parameters and their uncertainties change. During operation, fuel composition will change as the effect of depletion causing new actinide isotopes to appear [10]. This will contributes to delayed neutron emission, and affect the energy produced by the reactor. Figure 8 shows the fuel burn-up of each core. From (a) it can be seen that core1 and core2 have the same burn-up for uranium fuel, starting at 500 MWD/Ton and raising until >10.000 MWD/Ton at the core EOL. This number is smaller compared to figure (b), with core2 at the highest peak burning approximately 17.000 MWD/Ton, but still higher than core1 (<8000 MWD/Ton). In figure (b) we can see that when the reactor is operating, core2 will burn more fuel than core1.

5. Conclusion
We investigated the nuclear data of 2-region Th-U\textsuperscript{233} and Th-Pu MSR with the fuel cycle set to 21 each for 100 days. FUJI-U2 that was proposed by Y.Honma et al., is adopted as the MSR design. There are some discrepancies from the reference study and the simulation result regarding the K-\textit{inf} and K-\textit{eff} value, which suspected to be caused by different JENDL usage. Data concerning burn-up, conversion ratio, and elemental composition are also discussed and analyzed. When use as fuel, uranium and plutonium showed a unique profile and from the study it is concluded that adjustments is necessary for the proposed Th-Pu fuel mixture to sustain the reactor stability.

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